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(71) Applicant *(for all designated States except US)*: **ISIS INNOVATION LIMITED** [GB/GB]; Ewert House, Ewert Place, Summertown, Oxford, Oxfordshire OX2 7SG (GB).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **CERUNDOLO, Vincenzo** [IT/GB]; Institute of Molecular Medicine, University of Oxford, John Radcliffe Hospital, Oxford, Oxfordshire OX3 9DS (GB). **GADOLA, Stephan** [CH/CH]; Department of Rheumatology and Clinical Immunology, University of Berne, Inselspital, CH-3010 Berne (CH).

(74) Agents: **CRIPPS, Joanna, E.** et al.; Mewburn Ellis, York House, 23 Kingsway, London, Greater London WC2B 6HP (GB).

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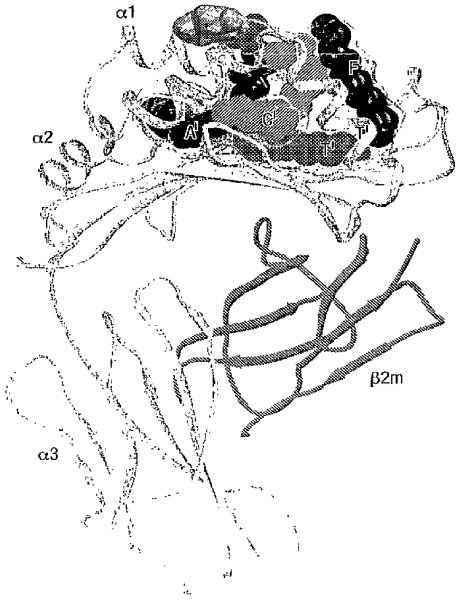

(57) Abstract: The present invention relates to methods of producing CD1/ligand complex comprising the steps of (a) obtaining a denatured CD1 protein; (b) contacting the denatured CD1 protein with ligand in an environment comprising detergent; and (c) isolating the CD1/ligand complex. The invention further relates to uses of obtained CD1/ligand complex, the crystal structure thereof and to computer-based methods and systems for rational drug design, assessment of candidate modulator molecules and methods for determining homologous or analogous protein structures.

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Immunogenic Complexes

Field of the Invention

The present invention relates to immunogenic complexes. Particularly, but not exclusively, the present invention relates to the production and use of type II glycoproteins displaying glycolipid and phospholipid antigens.

Background of the Invention

The CD1 gene cluster on human chromosome 1q22-23 encodes a family of five type II glycoproteins which are expressed on the cell surface in association with beta-2-microglobulin (β2m). According to their amino acid sequence homology the five CD1 isoforms segregate into group 1, containing CD1a, b, c, and CD1e, and group 2, containing CD1d. While CD1 group 1 molecules are not present in mice and rat, CD1d is conserved in all mammalian species studied to date.

In contrast to the highly polymorphic HLA class I and class II molecules, with which they share a common genetic ancestor, CD1 molecules are non-polymorphic. It was probably for this reason, that their role as antigen presenting molecules remained unrecognised for more than a decade after their initial description. The lack of polymorphism indicates that, as opposed to HLA class I and class II genes, the CD1 genes are subjected to very weak evolutionary pressure. Two features of CD1 molecules offer an explanation for this phenomenon. Firstly, CD1 molecules do not present peptides as HLA class I and HLA class II molecules do, but they present glycolipids and phospholipids to T lymphocytes. Immune escape of microbes

from HLA class I or class II-mediated responses can simply be achieved with functionally irrelevant changes in protein sequences abrogating binding and/or presentation of immunogenic peptides.

In contrast, lipid antigens cannot be easily mutated because lipids are end products of highly complex biosynthetic pathways, and because their physicochemical properties, which are essential to the organism, rely on their correct structure.

A second characteristic of CD1 molecules, which could also lower the ligand-induced evolutionary pressure on CD1, is their apparent high degree of ligand binding adaptability. In particular, human CD1b can present the carbohydrate epitope of either a mycobacterial derived eighty carbon containing (C80) glucomonomycolate (GMM) or a shorter thirty-two carbon (C32) synthetic GMM to the same T cell receptor, suggesting either adaptive conformational changes within the CD1 antigen binding groove or simply protrusion of the longer alkyl chain of the ligand at one end of the groove. The crystal structure of mouse CD1d, which was determined in the absence of ligand, revealed two electrostatically neutral voluminous pockets A' and F', suited to bind the alkyl chains of CD1 lipid ligands.

However, it is still completely unknown how different lipid classes bind to the CD1 groove, and how the same CD1 binding pocket can accommodate alkyl chains of different lengths. Furthermore, while a common motif for CD1b and CD1d-binding ligands has been proposed, consisting of a single proximal branched acyl chain or

two acyl chains, another CD1-molecule with high predicted structural similarity to CD1b, namely CD1c, presents single alkyl chain containing polyprenols to T cells. Moreover, recent evidence indicates, that single alkyl chain lipids can also be bound and presented by CD1d.

WO 01/94949 relates to compositions and methods for identifying CD1-antigens and CD1-restricted T cells. The compositions include soluble CD1 molecules. A method for identifying a CD1-restricted T cell comprising contacting a CD1-presented antigen complex with a putatative CD1-restricted T cell is disclosed.

WO 96/12190 relates to the presentation of hydrophobic antigens to T-cells by CD1 molecules and discloses the identification of human CD1a, CD1b, CD1c, CD1d and CD1e.

WO 95/00163 relates to a method for isolating CD1-presented antigens from a sample.

In "Presentation of the same glycolipid by different CD1 molecules" A.Shamshiev *et al* J.Exp. Med (April 15, 2002), 195(8), pp.1013-1021, the authors conclude that group I CD1 molecules present an overlapping set of self-glycolipids.

Summary of the Invention

To elucidate the mechanisms and potential of lipid binding to CD1 the inventors attempted to crystallise human CD1b with bound ligand. They found that in order to ensure binding of only their chosen ligands to CD1, they had to develop a novel detergent-assisted protocol to

refold CD1b in vitro from completely denatured and reduced E.coli derived protein.

The inventors subsequently obtained two crystal structures of human CD1b, one with phosphatidylinositol (PI) at 2.26Å and another with ganglioside GM2 at 2.8 A. The mode of ligand binding was almost identical for both structures. Interestingly, the C16 alkyl chain detergent used in the inventor's refolding protocol acted as an additional ligand in both structures by binding to those areas of the CD1b-binding groove that were not occupied by the glycolipid or phospholipid ligands.

Furthermore the inventors generated fluorescent tetramers of human CD1d molecules loaded with the synthetic glycolipid alpha-galactosylceramide (aGC). These tetramers were shown by the inventors to specifically stain a human immunoregulatory T-lymphocyte population, i.e. invariant NKT cells.

Thus, at its most general, the invention provides a method for producing a CD1/ligand complex; methods of diagnosing or treating patients using said CD1/ligand complex; and screening methods for determining new therapeutic targets on the CD1 complex, following determination of its crystal structure.

Accordingly, in a first aspect, there is provided a method of producing correctly folded recombinant CD1 molecules around various lipid ligands, such as gangliosides, phospholipids and glycosylceramides. The resulting CD1/ligand complex is biologically active, i.e. the ligand is displayed correctly by the CD1 molecule so

that it can be presented to immune components, e.g. T lymphocytes.

In the past, CD1a and CD1b have been successfully refolded using immobilised enzymes. However, there was no evidence of ligand being present in the refolded molecules. As mentioned above, the inventors have devised a novel approach using single chain detergents. This approach is inexpensive and can easily be scaled up for industrial purposes. The inventors have further provided direct evidence that the lipid ligand is bound to the hydrophobic groove of CD1 molecules.

Thus, in accordance with the first aspect of the invention, there is provided a method of producing a CD1/ligand complex said method comprising the steps of:

a) obtaining a denatured CD1 protein;

b) contacting said denatured CD1 protein with ligand in an environment comprising detergent; and

c) isolating said CD1/ligand complex.

Preferably, the CD1 protein is fully denatured and reduced to ensure that the protein is unfolded when initially contacted with ligand. Although it is preferable to also reduce the protein, the presence of native disulfide bridges would not prevent the protein from refolding with ligand. However, when expressed as inclusion bodies in E.coli, correct or native formation of disulfide bridges cannot be presumed. Proteins with incorrect disulfide bridges will not fold correctly and could potentially reduce the efficacy of in vitro refolding of other protein by increasing the tendency of protein-protein aggregation.

The ligand may be any lipid, but most preferably, it is a glycolipid (e.g. ganglioside GM2 or alpha-galactosylceramide) or phospholipid (e.g. phosphatidylinositol). The inventors have determined that the CD1 molecule is capable of displaying lipids of various sizes. Thus, for a single chain ligand the molecule is preferably anything up to 60 carbons in length, e.g. between 5, 10 or 15 and 30, 40 or 50 carbons in length. For a double chain ligand, the molecule may contain anything between 18 carbons to 100 carbons, e.g. between 10, 20, 30 or 40 and 70, 80, or 90 carbons in length.

Preferably, the detergent is a single chain detergent, such as acyclic single alkyl chain detergents with chain length C2-C60; sphingosines; ceramides with truncated alkyl chains; diacylglycerol-type lipids with truncated alkyl chains; and triacylglycerol-type lipids with truncated alkyl chains. The inventors favoured the use of cetyltrimethylammonium bromide (CTAB).

The method preferably further comprises the step of removing excess detergent from the environment prior to isolation of the CD1/ligand complex. The excess detergent which has not stably incorporated into the protein structure, may be removed by adding methylated or unmethylated beta-cyclodextrin in molar excess over detergent. The inventors prefer to use at least 12 molar excess of methyl-beta-cyclodextrin. However, other methods will be known to the person skilled in the art. For example, other cyclodextrins (alpha and gamma) which vary in the size of their hydrophobic cavity. The

inventors preferred methyl-beta-cyclodextrin but other cyclodextrins will work in accordance with the invention. Other methods for stripping off the excess detergent include the use of resins or dialysis.

It is preferred to use a step that allows rapid stripping of the detergent as slow removal by resins or dialysis may decrease the yield of the CD1/ligand complex.

The method according to the first aspect of the invention may be carried out using any CD1 molecules. However, preferably, the method is carried out on CD1d, CD1c and most preferably on CD1b.

The environment comprising the detergent will also comprise various buffers to aid in the refolding event. Preferably, an aqueous buffer is provided comprising Urea, L-Arginine, a buffer (e.g. Tris), and a redox-system (e.g. oxidized and reduced glutathione). The buffer constituents can be varied: L-Arginine can be used in various concentrations from 100mM, preferably at a concentration between 100mM to 1M, but may not even be essential to get a certain yield of refolded CD1. The same applies for Urea, which can certainly be used in concentrations ranging from 0M to 4M. At the higher concentrations a dialysis step may be necessary. Instead of glutathione another redox system such as cysteamine-cystin, could be used and the molarities of glutathione can be varied.

The CD1 protein may be engineered to contain one or more biotinylation sites providing a means for complexing CD1 proteins using avidin to obtainmultimeric, e.g. dimer,

trimer, tetramer, forms of CD1 which may be useful in amplifying output signals in methods and assays for identifying ligand specific T-cells or antibodies.

In preferred arrangements, the CD1 protein may be complexed with the Fc portion of a selected immunoglobulin. The complex may be formed by using binding partners (biotin - avidin) or by chemical means (covalent, di-sulfide, H-bonds).

Preferably, the method of the first aspect may further comprise the step of labelling the CD1 protein with a chemical marker, more preferably a fluorescent compound, e.g. RPE or FITC. The labelled CD1 protein useful in identification of specific T-cell populations and for diagnosis of specific disease states. In particular, mulitmers, e.g dimers, trimers or tetramers, of labelled CD1/ligand complex may be used.
The method may further comprise the step of incorporating said CD1/ligand complex into a pharmaceutical composition. The pharmaceutical composition may comprise, in addition to one of the above substances, a pharmaceutically acceptable excipient, carrier, buffer, stabiliser or other materials well known to those skilled in the art. Such materials should be non-toxic and should not interfere with the efficacy of the active ingredient. The precise nature of the carrier or other material may depend on the rate of administration, e.g. oral, intravenous, cutaneous or subcutaneous, nasal, intramuscular, intraperitoneal routes.

In an embodiment of the present invention, the pharmaceutical composition may be used as a vaccine to

boost the immune response in an individual. Thus, it is preferable that the composition further comprises a suitable adjuvant. The pharmaceutical composition according to the present invention may be used to elicit cellular immune responses including lipid-specific $CD4^+CD8^-$, $CD4^-CD8^+$, and $CD4^-CD8^-$ T cell responses. Alternatively, antibody responses to the pharmaceutical composition would also be of therapeutic value.

The present invention provides a pharmaceutical composition comprising a CD1/ligand complex for treating diseases such as infectious diseases caused by parasites, mycobacteria, fungi, and bacteria; tumours and autoimmune diseases such as multiple sclerosis.

Depending on the disease to be treated, the ligand will be a lipid that is capable of inducing an immune response, against substances (e.g. tumour cells, bacteria, myobacteria etc.) associated with the disease. For example, ligands may be

a) Mycobacterial cell wall lipids: Glycosyl-esters of mycolic acid (glucomonomycolate, mannose-monomycolate, etc.) Phosphatidylinositomannosides (PIM2 to PIM6), as well as synthetic lipids modelled after mycobacterial cell wall lipids (synthetic glucomonomycolate, etc.)

b) ganglioside lipids such as GM1 or GM2 or GM3, etc.; Also diacylglycerol-type bacterial cell wall lipids;

c) sulfatide;

d) trypanosomal phospholipids; malarial cell wall lipids.

For the treatment of tumours, ligand may be lipids expressed on the surface of tumour cells.

Thus, embodiments of the present invention provide a CD1/ligand complex for use in the preparation of a medicament for treating infectious diseases caused by parasites, mycobacteria, fungi, and bacteria; solid tumours; and autoimmune diseases. In preferred embodiments use of a CD1/ligand complex produced in accordance with the first aspect of the invention and a method of medical treatment comprising administering the CD1/ligand complex in therapeutically effective amounts are provided.

In accordance with a second aspect of the present invention, there is provided a method of inducing or boosting an immune response in an individual to a lipid antigen, said method comprising administering a CD1/ligand complex to said individual wherein the ligand in the CD1/ligand complex is said lipid antigen.

The CD1/ligand complex may be produced according to the first aspect of the invention.

The method may further comprise identifying the lipid antigen associated with a disease of the individual, i.e. cancer, infectious disease or autoimmune disease.

For example, the method may comprise identifying a lipid antigen over-expressed on the surface of tumour cells present in the individual. The identified lipid antigen may then be folded into a CD1 molecule in accordance with the first aspect of the invention thereby producing a

CD1/ligand complex which may be administered as a vaccine to said individual to raise an immune response against said tumour.

With regard to autoimmune diseases, the CD1 ligand complex may further comprise a toxin which is capable of disrupting an immune response raised against the lipid antigen. For example, the provision of a toxin-conjugated CD1/ligand complex may be used to eliminate specific T lymphocytes which interacted with the complex. Autoimmune T lymphocytes represent a therapeutic target for such toxin-conjugated CD1/ligand complexes.

In a third aspect of the present invention, the CD1/ligand complex according to the present invention may also be used to diagnose a disease in an individual, by identifying the presence or absence of an immune response, i.e. CD/1 lipid-specific T-lymphocytes or antibodies, to a particular lipid antigen. Thus, a sample may be obtained from an individual, and contacted with a CD1/ligand complex of the invention. If the CD1/ligand complex was being used to identify the presence of an autoimmune disease, the complex would display a lipid antigen associated with this disease. If the sample comprised T-lymphocytes or antibodies already primed to the lipid antigen, these will be detected by the CD1/ligand complex contacted with the sample. Standard labelling techniques may be used to identify any binding between the CD1/ligand complex and the immune components in the sample.

In accordance with any of the aspects described above, the CD1/ligand complex may be provided as a monomer,

dimer, trimer, tetramer etc. Complexes may be joined by standard means known in the art, e.g. using binding partners (biotin - avidin) or chemical means (co-valent, di-sulfide, hydrogen bonds), so that the ligand is displayed and could be recognised by the T cell receptor.

According to a fourth aspect of the present invention, the inventors have prepared a crystal of CD1/ligand complex and determined the crystal structure of CD1 and CD1/ligand complex. This provides for the first time methods of identifying or obtaining substances (e.g. agonists or antagonists) for modulating the activity of CD1 or CD1/ligand complex. Crystal structure information presented herein is useful in designing potential inhibitors and modelling them or their potential interaction with a CD1 or CD1/ligand complex binding cavity.

Potential modulating substances may be brought into contact with CD1 or CD1/ligand complex to test for ability to interact with the CD1 binding cavity. Actual substances may be identified from among potential substances synthesized following design and model work performed *in silico*. A substance identified using the present invention may be formulated into a composition, for instance a composition comprising a pharmaceutically acceptable excipient, and may be used in the manufacture of a medicament for use in a method of treatment.

Thus, in the fourth aspect of the invention, there is provided a crystal of CD1 and CD1/ligand complex. Preferably, the ligand is a lipid, more preferably a glycolipid or a phospholipid. The crystal may have unit

cell dimensions of a = 87.5 Å ± 5%, b = 177 Å ± 5% c = 75 Å ± 5%.

Preferably a = 87.5 Å ± 0.2%, b = 177 Å ± 0.2 % c = 75 Å ± 0.2%.

In a preferred embodiment, the crystal structure of CD1 and CD1/ligand complex has the three dimensional atomic co-ordinates of Table 1.

In a preferred embodiment the ligand is phosphatidylinositol (PI) or ganglioside GM2 and the CD1 molecule is CD1b, CD1c or CD1d, preferably CD1b.

A method for growing the crystal of the fourth aspect by sitting drop crystallisation using a precipitant comprising 0.2M Lithium nitrate and 20% w/v Polyethylene Glycol is also provided.

The coordinates of Table 1 provide a measure of atomic location in Angstroms (Å), to a third decimal place. The coordinates are a relative set of positions that define a shape in three dimensions, but the skilled person would understand that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Furthermore, the skilled person would understand that varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for

the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and potency for structure-based design of CD1 inhibitors. Likewise the skilled person would understand that changing the number and/or positions of the water molecules and/or substrate molecules of Table 1 will not generally affect the potency of the structure for structure-based design of CD1 inhibitors. Thus for the purposes described herein as being aspects of the present invention, it is within the scope of the invention if: the Table 1 coordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structure are varied so that the root mean square deviation of residue backbone atoms is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the coordinate data of Table 1 thus includes the coordinate data in which one or more individual values of the Table are varied in this way. By "root mean square deviation" we mean the square root of the arithmetic mean of the squares of the deviations from the mean.

Thus, for example, varying the atomic positions of the atoms of the structure by up to about 0.2 Å in any direction will result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and utility e.g. for structure-based drug design.

The provision of the high resolution structure of Table 1 provides those of skill in the art with a detailed insight into the mechanisms of action of CD1 or CD1/ligand complex. This insight provides a means to design new substances which have the potential to modulate, e.g. inhibit or enhance the process by which CD1 presents ligand to the immune system.

The provision of the crystal structure of CD1 and CD1/ligand complex allows a novel approach for drug discovery for modulators of this enzyme. Accordingly, in a fifth aspect of the invention a computer-based method of rational drug design is provided comprising the steps of:

providing the structure of the CD1 or CD1/ligand complex as defined by the coordinates of Table 1;

providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the structure of the CD1 or CD1/ligand complex of Table 1.

In an alternative aspect, the method of the invention may utilise the coordinates of atoms of interest of the CD1 which are in the vicinity of a putative ligand pocket in order to model the pocket in which the ligand fits. These coordinates may be used to define a space which is then screened *"in silico"* against a candidate modulator molecule. Thus, in a sixth aspect, the invention provides a computer-based method of rational drug design which comprises:

providing the coordinates of at least two atoms of

the CD1 of Table 1 ("selected coordinates");

providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the selected coordinates of the CD1.

In practice, it will be desirable to model a sufficient number of atoms of the CD1 as defined by the coordinates of Table 1 which represent a binding pocket e.g. A' C' F' or T'.

Thus preferably there will be provided the coordinates of at least 5 or 10, more preferably at least 50 and even more preferably at least 100 selected atoms of the CD1 structure.

Preferably, the invention also relates to fragment linking or fragment growing approaches to rational drug design. Thus the step of providing the structure of a candidate modulator molecule may be performed by providing the structures of a plurality of molecular fragments and linking the molecular fragments to form a candidate modulator molecule. Furthermore the step of fitting the structure of the candidate modulator molecule may be performed before the molecular fragments are linked together, by separately fitting the structure of each molecular fragment, or after the molecular fragments are linked together.

Thus, the computer-based method of rational drug design may comprise:

providing the coordinates of at least two atoms of the CD1 or CD1/ligand complex of Table 1;

providing the structures of a plurality of molecular fragments;

fitting the structure of each of the molecular fragments to the selected coordinates of the CD1 or CD1/ligand complex; and

assembling the molecular fragments into a single molecule to form a candidate modulator molecule.

In one embodiment, the computer-based method may further comprise the steps of:

obtaining or synthesising the candidate modulator molecule;

contacting the candidate modulator molecule with CD1; and

determining the ability of the candidate modulator molecule to interact with CD1.

In another embodiment, the computer-based method may further comprise the steps of:

obtaining or synthesising the candidate modulator molecule;

forming a complex of CD1 and said candidate modulator molecule; and

analysing said complex by X-ray crystallography to determine the ability of said candidate modulator molecule to interact with CD1.

A further aspect of the invention provides a compound having a chemical structure selected using the method of any one of the previous aspects, said compound being a modulator of the activity of CD1, e.g. an inhibitor or enhancer of CD1 ligand presentation.

The step of providing the structure of a candidate modulator may involve selecting the compound by computationally screening a database of compounds for interaction with the active site. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the active site. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor is a type of virtual pharmacophore.

In any event, the determination of the three-dimensional structure of CD1 and CD1/ligand complex provides a basis for the design of new and specific ligands for CD1 or modulators of CD1 activity. For example, knowing the three-dimensional structure of CD1/ligand complex, computer modelling programs may be used to design different molecules expected to interact with possible or confirmed active sites, such as binding sites or other structural or functional features of CD1.

More specifically, a potential modulator of CD1/ligand complex activity can be examined through the use of computer modelling using a docking program such as GRAM, DOCK, or AUTODOCK (see Walters et al., *Drug Discovery Today*, Vol.3, No.4, (1998), 160-178, and Dunbrack et al., *Folding and Design*, 2, (1997), 27-42).

Accordingly, in a seventh aspect, the present invention provides a machine readable data storage medium comprising a data storage material encoded with machine

readable data, wherein the data is defined by all or a portion of the structure coordinates of CD1/ligand complex according to Table 1. The invention further includes use of the machine readable data storage medium to design modulators of the CD1/ligand complex.

In an eighth aspect of the invention, there is provided a computer system intended to generate structures and/or perform rational drug design for CD1/ligand complex, or complexes of CD1/ligand with a potential modulator, the system containing machine readable data comprising:
(1) atomic coordinate data of Table 1, said data defining the three dimensional structure of CD1/ligand complex, or at least one sub-domain of the three-dimensional structure of CD1/ligand complex, or the coordinates of at least two atoms of CD1/ligand complex; or
(2) structure factor data for CD1/ligand complex, said structure factor data being derivable from the atomic coordinate data of Table 1.

Having designed or selected possible binding candidate modulators (e.g. by *in silico* analysis, "wet" chemical methods, X-ray analysis etc.) by determining those which have favourable fitting properties (e.g. strong attraction between candidate and CD1), these can then be screened for activity. Consequently, the method preferably further comprises the steps of:

obtaining or synthesising the candidate modulator; and

contacting the candidate modulator with CD1/ligand complex to determine the ability of the candidate modulator to interact with CD1/ligand complex.

More preferably, in the latter step the candidate modulator is contacted with CD1/ligand complex under conditions to determine its function.

Following identification of a modulator (e.g. an enhancer or inhibitor), it may be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

In a ninth aspect, the present invention provides a method for identifying a candidate modulator (e.g. potential enhancer) of CD1/ligand complex comprising the steps of:

providing the three-dimensional structure of CD1/ligand complex, or at least one sub-domain thereof, to characterise at least one active site of CD1, the three-dimensional structure being defined by atomic coordinate data according to Table 1; and

identifying a candidate modulator molecule for interaction with the active site. Preferably, the candidate modulator molecule is identified by designing or selecting the molecule to interact with the active site.

If more than one CD1 active site is characterised and a plurality of respective compounds are designed or selected, the modulator may be formed by linking the respective compounds into a larger compound which maintains the relative positions and orientations of the respective compounds at the active sites. The larger

compound may be formed as a real molecule or by computer modelling.

Preferably, high throughput screening of compounds to select compounds with binding activity may be undertaken, those compounds showing binding activity being selected as possible candidate modulators, and further crystallized with CD1 (e.g. by co-crystallization or by soaking) for X-ray analysis. The resulting X-ray structure may be compared with that of Table 1 for a variety of purposes. For example, where the contacts made by such compounds interact with a plurality of active sites, e.g. where the contacts overlap with those made by lipid antigen, novel molecules comprising residues contacting both lipid antigen and the bound compound may be obtained.

Identified modulators (e.g. an enhancers or inhibitors), may then be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

A tenth aspect of the present invention provides a method of assessing the ability of a candidate modulator molecule to interact with CD1 or CD1/ligand complex comprising the steps of:

obtaining or synthesising said candidate modulator molecule;

forming a crystallised composite of CD1 or CD1/ligand complex and said candidate modulator; and

analysing the composite by X-ray crystallography to determine the ability of the candidate modulator to interact with CD1 or CD1/ligand complex.

Preferably, the composite diffracts X-rays for the determination of atomic coordinates of the composite to a resolution of better than 3Å, more preferably better than 2Å. The crystallised composite may be formed by crystal soaking or co-crystallisation.

By utilising the high resolutions obtainable with X-ray crystallography, it is possible to determine the ability of the candidate modulator molecule to interact with CD1 or CD1/ligand complex by comparing the intensities and/or positions of X-ray diffraction spots from the composite with diffraction spots of uncomplexed CD1 or a previously identified CD1/ligand complex. Thus, the step of analysing the composite may involve analysing the intensities and/or positions of X-ray diffraction spots from the composite to determine the ability of the candidate modulator molecule to interact with CD1 or CD1/ligand complex.

In another aspect, the invention relates to a method of determining three dimensional structures of CD1/ligand complex homologues or analogues of unknown structure by utilising the structural coordinates of Table 1.

For example, if X-ray crystallographic or NMR spectroscopic data is provided for a CD1 homologue or analogue of unknown structure, the structure of CD1 as defined by Table 1 may be used to interpret that data to provide a likely structure for the CD1 homologue or

analogue by techniques which are well known in the art, e.g. phase modelling in the case of X-ray crystallography.

Thus, in an eleventh aspect of the present invention a method of determining three dimensional structures of CD1 or CD1/ligand complex homologues of unknown structure is provided, comprising the steps of:

aligning a representation of an amino acid sequence of a CD1 or CD1/ligand complex homologue or analogue of unknown structure with the amino acid sequence of CD1 or CD1/ligand complex to match homologous regions of amino acid sequences;

modelling the structure of the matched homologous regions of the homologue or analogue of unknown structure on the structure as defined in Table 1 of the corresponding regions of CD1 or CD1/ligand complex; and

determining a conformation for the homologue or analogue of unknown structure which substantially preserves the structure of said matched homologous regions.

Preferably, said homologues have an amino acid sequence having at least 50% homology with said CD1, more preferably at least 60%, 70%, 80% or 90% homology.

In a twelfth aspect of the present invention there is provided a method for determining the structure of a protein comprising the steps of:

providing the coordinates of Table 1; and

either (a) positioning said coordinates in the crystal unit cell of said protein so as to provide a

structure for said protein, or (b) assigning NMR spectra peaks of said coordinates.

In a thirteenth aspect of the present invention there is provided a method for determining the structure of a compound bound to CD1/ligand complex comprising the steps of:

providing a crystal of CD1/ligand complex; and

soaking the crystal with the compound to form a complex; and

determining the structure of the complex by employing the data of Table 1.

Aspects and embodiments of the present invention will now be illustrated, by way of example, with reference to the accompanying figures. Further aspects and embodiments will be apparent to those skilled in the art. All documents mentioned in this text are incorporated herein by reference.

Brief Description of the Drawings

Figure 1: Structure of the human CD1b complex and of its ligands. **a**, CD1b structure (α1-α3 domains in light shading, β2m in dark shading with left to right hatching) with bound PI (alkyl chains in grey shading with right to left hatching (C') and dark shading (A'), inositol dot filled in light grey and adjacent phosphate dot filled in black) and detergent molecules (dark shading (F') and dot filled in black (T')) shown as Van Der Waals spheres. The internal hydrophobic cavity of α1α2 is drawn as a transparent surface, and ligand binding channels are indicated as A', C', F' and T'. **b**, Chemical structures of

lipid and detergent ligands used in the refolding of CD1b complexes.

Figure 2: Binding and presentation of alkyl chain ligands by CD1b. All panels depict the CD1b/PI complex excepting **b** and **c** which show CD1b/GM2. **a**, Overview of the α1α2 domain of CD1b with bound ligands. Close up views of the framed regions of the groove are shown in panels **b-g**. **b** and **c**, Positioning of the first glucosyl- and the phosphoinositol head groups in the CD1b-GM2 and CD1b-PI structures, respectively. Carbon atoms of the lipid ligand are grey shaded with right to left hatching, oxygens are black spheres, phosphate is hashed, and nitrogen dot filled black. Hydrogen bonds are shown as black dotted line. **d**, The F′channel with bound monoalkyl detergent. **e**, A single detergent molecule bound to tunnel T′ traverses a path, unobstructed by bulky side chains, between channels A′ and F′. **f**, A portal in the C′channel, stabilised by a unique disulfide bond Cys131-Cys145 (square dot infill) , allows egress of the lipid from the interior of the protein. **g**, The bottom of the A′channel contains a hydrophobic pole formed by Val12 and Phe70, which could guide the lipid ligand from the A′ channel into the T′ tunnel. In all panels, the F_o-F_c omit map electron density (thin line mesh, contoured at 2.5σ) was calculated after a simulated annealing during which the glycolipid (plus any residues and detergent within a distance of 3.5Å) were omitted, in panels **d-g**, the 2 F_o-F_c Φ_{calc} electron density of the protein structure is shown as a white surface, contoured at 1σ.

Figure 3: Differences between CD1b and other CD1 isoforms. **a, b,** Structural comparison of the antigen binding cavity for hCD1b and mCD1d. The hydrophobic groove and key side chains of CD1b and CD1d are shaded. The ligands present in the CD1b structures were superimposed onto the mCD1d structure for direct comparison. **c,** Sequence alignment of the α1α2 domains of human CD1a-e and mCD1d. Secondary structure elements of CD1b are shown above the protein sequence. A shaded background indicates those residues which confer the lipid binding properties of CD1b and which are conserved at equivalent positions in other CD1 isoforms. Hydrophobic residues guiding the lipid ligands in CD1b at the bottom of channel A′ (see Fig. 2g) and between channels C′ and F′ are indicated by triangles, respectively. Cysteine residues are boxed.

Figure 4: Models for binding of mycolic acid and triacylglycerol to CD1b. **a,** Chemical structures of mycolic acid from *M.tuberculosis* and of the triacylglycerol trilaurin. **b,** Mycolic acid modeled into the CD1b structure. The C60 long meromycolate chain (hash infill) could be fully contained within channels A′, T′ and F′, thus forming a superchannel of some 70Å length. The shorter C25 alkyl chain (dark shaded) is therefore more likely to lodge in the C′ channel. **c,** Model of triacylglycerol (trilaurin) binding to CD1b, demonstrating that the three C11 alkyl chains (dot infill) could separately bind to surface-linked channels A′, C′ and F′. To demonstrate the full binding potential of the CD1b groove, alkyl chains present in the CD1b-PI and CD1b-GM2 structures but not accounted for by the models are overlayed in light grey. Conversely,

polycarbon chains, which the crystal structures provide no models, are indicated by dotted lines.

Figure 5: CD1d/aGC complexes are specific for human invariant NKT cells. Use of fluorescent CD1d/aGC tetramers as a diagnostic composition in identifying human invariant NKT cells by FACS analysis. **a**, FSC-H/SSC-H plot used for gating of lymphocyte population. **b**, Propidium iodide staining gates out dead cells. **c**, Staining of human invariant NKT cells with anti-T-cell receptor (anti-TCR) Valpha24 antibody. **d**, **e**, CD1d/aGC tetramers stain human invariant NKT cells.

Detailed Description

Compared to in vivo folding, in vitro folding of proteins is generally much less effective. Mammalian cells possess a range of specialised helper proteins, e.g. chaperonins, disulfidases, proline isomerases, etc., which enhance the yield of correctly folded molecules. Standard in vitro refolding protocols, which were successful for HLA class I molecules were completely unsuccessful for refolding CD1 molecules. As CD1 molecules are significantly more hydrophobic than HLA class I molecules, the inventors thought that the difficulties with standard protocols were due to hydrophobic interactions between partially folded CD1 molecules, causing the proteins to aggregate and precipitate. When a fully denatured protein starts to fold, it goes through a transition state, hydrophobic residues are exposed to the surroundings, and if two proteins meet, they will bind to each other and precipitate. To overcome this possible problem, the inventors used single chain detergents as folding assistants. The idea was that detergent molecules and

folding CD1 molecules would form mixed detergent-protein micelles which would allow the proteins to proceed with the folding beyond the molten-globule state, while being physically separated from each other.

The second stage of the process is to strip off the detergent from these micelles so as to allow the molecules to completely fold. The detergent is stripped using, for example, soluble cyclodextrins.

The inventors have been able to crystallise CD1b molecules generated by this method and have obtained high resolution structure of CD1b with bound ligand. The crystal structure revealed that the large groove of Cd1b is not only occupied by ligand but also by the detergent molecule.

The ligand is loaded in a way that allows optimal presentation of the antigenic epitope to the T cell receptor, while two detergent molecules per CD1 molecule fill the rest of the large groove. Thus, in accordance with the present invention, the loaded CD1 molecule (CD1/ligand complex) is considered biologically active.

As an example of the present invention, the inventors have refolded the extracellular region of human CD1b (hCD1b; heavy chain residues 1-283 plus beta-2-microglobulin, β2m) *in vitro* from completely denatured and reduced E.coli-derived proteins. Single alkyl chain detergents of sixteen carbon length (C16) were used as refolding assistants to protect exposed hydrophobic surfaces during early refolding stages, thereby reducing hydrophobic protein aggregation and precipitation. This

protocol yielded stable soluble CD1b/β2m-complexes, which mass spectrometry confirmed to be loaded with the specified lipid ligands plus detergent (see methods).

Soluble CD1b/β2m-proteins loaded either with phosphatidylinositol (PI) or ganglioside GM2 (GM2)[8] were crystallised, their structures determined by molecular replacement and refined using data to 2.26Å and 2.8Å, respectively (see Fig. 1, 2, methods and supplementary information).

The CD1b heavy chain and β2m structures are identical in the two complexes and unless otherwise stated the following analyses are based on the higher resolution CD1b/PI structure. The structures reveal a defined network of hydrophobic channels at the core of the α1α2 domain which are precisely tailored for acyl binding and are saturated by four hydrocarbon chains of 11 to 22 carbon atoms in length. This binding groove architecture is radically different to that of classical MHC class I and II molecules. The total volume (2200Å^3) of the network is essentially filled by the hydrocarbon chains. No buried water molecules are present in either structure. In an extension of the analogy with MHC class I binding pocket nomenclature introduced for mCD1d[7], the three CD1b binding channels which connect directly to the surface are denoted as A′, C′ and F′, with the fourth, a unique tunnel, designated T′ (Fig. 1, 2). Channels A′, C′, and F′ interconnect via T′. The sequential connection of A′, T′ and F′ provides the potential to accommodate up to 60 carbon atoms of a single acyl chain which could enter and exit between the α1 and α2 helices (along A′ and F′). Channel C′ remains separate, leading from the T cell

receptor (TCR) recognition surface between the α1 and α2 helices to a portal in the side of the molecule beneath the α2 helix (Fig 1, 2d). Thus this channel can shelter acyl chains of some 16 carbon atoms fully from solvent whilst allowing egress for longer chains. The PI and GM2 ligands occupy channels A′ and C′, whilst two detergent molecules fill channels F′ and T′ (Fig. 1, 2, 3). There is sufficient electron density to position unequivocally the link between the acyl chains and hence partial head-group structures for the glycolipids in the CD1b/GM2 and CD1b/PI complexes (Fig. 1, 2a, 2b). The inositol ring of PI is partially ordered in the CD1b/PI complex, whilst only the first of the four sugar rings which branch off the GM2 lipid head is visible in the CD1b/GM2 crystal structure. Comparison with a classical MHC class I/peptide complex shows the glycolipid head groups to be presented by CD1b in a position analogous to that of the P4 residue in a peptide presented by MHC class I. The surface presented by the CD1b/glycolipid complexes appears compatible with standard TCR recognition, a conclusion borne out by mutagenesis studies mapping TCR binding to CD1b[9]. In contrast, key features of the α3 domain required for MHC class I binding to CD8 are not conserved in CD1b[10].

Comparison of the CD1b complexes with the structure of mCD1d, which does not include a specific bound ligand[7], indicates broad equivalences but also very significant differences in the architecture of the binding groove (Fig. 3). Channel A′ runs deeper in CD1b because Val63 replaces a bulky tryptophan at the equivalent position in mCD1d (additionally Ala47 is replaced by Ile). Channel T′, which in CD1b serves to connect channels A′ and F′,

is blocked in mCD1d by the side chains of Leu100 and Val118, equivalent to residues Gly98 and Gly116 respectively in CD1b. Similarly, the exit portal for channel C′ beneath the CD1b α2 helix (Fig. 2f) is closed off in CD1d by Phe128 and Trp133, being residues with bulky side chains, replacing Val126 and Cys131 respectively in CD1b. In CD1 alleles other than CD1b, the absence of a disulphide bridge (Cys 131 - Cys145, Fig 2f) pulls the α2 helix main chain more closely to the CD1 backbone. However, in addition to the differences hardwired by changes at sequence level the comparison of the CD1b and mCD1d structures also implies both molecules may share some conformational adaptability. While channel F′ is partially occluded in mCD1d by the side chain of Leu84 the side chain conformation selected by the equivalent residue (Phe84) in the current CD1b structure frees up sufficient space for F′ to accommodate a detergent molecule (Fig. 2d, 3). However, in the absence of ligand Phe84 may be expected to adopt an alternate conformation (analogous to that of Leu84 in mCD1d) to pack against Phe144, Phe88 and Met90. This suggests a mechanism whereby the hydrophobic binding capacity of the channels may be tailored to ligand requirements, a phenomenon previously observed for binding of non-nucleoside inhibitors to HIV Reverse Transcriptase[11].

The current CD1b structures allow definition of the residues which confer the lipid binding properties of the α1α2 domain. Sequence alignment of the CD1 family highlights channel A′ and the associated portion of tunnel T′ as the most conserved regions of the groove (Fig. 3c). Conversely, the central portion of tunnel T′ is blocked in all other CD1 isoforms by the presence of

bulky side chains of residues equivalent to Gly98 and Gly116 in CD1b. Similarly, the C′ portal is occluded by tryptophan and phenylalanine residues which substitute for CD1b residues Cys131 and Val126, respectively in all other CD1 family members. Residues contributing to channel F′ are least conserved. Overall, based on ligand binding architecture, CD1b appears to be unique among CD1 molecules.

The arrangement of the combined detergent and lipid ligands in the CD1b/PI and CD1b/GM2 structures provide a general model for describing the interaction of the CD1b-binding groove with alkyl chain containing ligands. Mycobacterial mycolates (Fig. 4a), which play a crucial role in the adaptation of mycobacteria to intracellular growth and survival[12], were the first fully characterised ligands of human CD1b[2]. It has long been speculated about how lipid ligands of such large size could bind to CD1b. Modelling of mycolic acid into the current CD1b structures demonstrates how the long C50-C56 meromycolate chain could be fully contained within a super channel consisting of the interconnected A′, T′ and F′ channels, with the shorter C22-C26 alkyl chain binding to C′ (Fig. 4b). The super channel has a maximum length of some 70Å providing binding capacity for a single fatty acid chain of up to 60 carbons. In the case of only partial saturation of the superchannel's alkyl binding capacity, the F′ channel could be closed off by selection of an alternative side chain conformation for Phe84 (see previously and Fig. 2d). This mechanism for adaptation to alkyl chain length would explain how CD1b can present either the large C80 mycobacterial glucomonomycolate or the shorter C32 synthetic glucomonomycolate to the same T

cell line[13]. The superchannel also allows for the option of stably accommodating long chain monoalkyl ligands, which can therefore serve as T cell antigens.

Short chain fatty acids of the endoplasmic reticulum, such as palmitate, could also act as ligands for CD1b in a similar manner to the C16 chain detergents used in the current refolding protocol (see methods). However, since the affinity of a given ligand to CD1b is related to the polycarbon chain length, endogenous short chain fatty acids could exert a chaperone-like function before binding of higher affinity ligands. Consistent with this hypothesis is the fact that, despite a 500 fold molar excess of detergent over lipid in the refolding buffer, detergent molecules were bound only to the T′ tunnel and F′ channel, while both the A′ and C′ channels were occupied by the two alkyl chains of the lipid ligand. This also suggests that surface CD1b molecules may still retain endogenous chaperones to account for any excess binding capacity, in particular in tunnel T′.

The arrangement of channels A′, C′ and F′ strongly suggests that lipids containing three alkyl chains, such as endogenous triacylglycerols or mycobacterial triacyl trehalose, may bind to human CD1b (Fig.4c). Triacylglycerols, which are synthesised on membranes of the endoplasmic reticulum, are independent risk factors for coronary heart disease[14, 15]. Activated memory T lymphocytes accumulate in atherosclerotic plaques[16, 17], and oxidized lipoproteins, which contain triacylglycerols, can act as immunogens for T cell[18, 19]. Interestingly, a recent study has found that CD1b is highly expressed on macrophages in atherosclerotic

lesions, but not on normal tissue macrophages[20]. It is therefore intriguing to speculate on the role of CD1b-mediated presentation of triacylglycerols to T lymphocytes in atherosclerosis.

The topology of CD1b is MHC class I-like (Fig. 1a) with close structural similarity to murine CD1d. Tubes of electron density (common to both the CD1b/GM2 and CD1b/PI structures) delineate binding channels, buried between the α1 and α2 helices, occupied by four acyl chains. These hydrocarbon chains are up to 80 carbon atoms in length. In the refined structures two of the acyl chains (in A′ and C′) are assigned to the tails of the glycolipid ligand and the remaining two (in F′ and T′) are accounted for by detergent molecules. Electron density at the CD1b surface linking chains A′ and C′ provide partial information for the position of the glycolipid head-group structures, which are relatively mobile as judged from crystallographic temperature factors.

The detergents used in the refolding of the single lipid complexes (see Methods) have supplemented GM2 and PI to saturate the acyl binding capacity of CD1b.

The structure of murine CD1d[7] does not include a specific bound ligand but the α1α2 domain contains cavities designated as binding pockets A′ and F′. Comparison with the CD1b complexes indicates broad equivalence of pocket A′ to channels A′ and of pocket F′ to channel F′. The CD1d cavities have a reduction in volume relative to the total CD1b network.

The main chain topology of CD1b differs markedly from MHC class I in the peak height attained by the kink in the α2 helix (residues 150-157 and 149-152 in CD1b and MHC class I respectively). Direct substitution of CD1b into a MHC class I/TCR complex (by simple superposition onto the MHC class I structure) therefore results in significant steric clashes between the TCR and this portion of the CD1b α2 helix. The upward displacement of the TCR necessary to provide a sterically acceptable dock onto the CD1b structure may facilitate incorporation at the recognition interface of the increased size of the glycolipid head group compared to an amino acid side chain. Given this modification the surface presented by the CD1b/glycolipid complexes appears compatible with standard TCR recognition, a conclusion borne out by mutagenesis studies mapping TCR binding to CD1. Superposition of CD1b into the HLA A2/CD8αα crystal structure[10] again reveals substantial steric clashes. Given the highly conserved nature of the MHC class I/CD8 interaction these changes imply relative abolition of any such interaction. This is again consistent with the functional recognition of CD1 by $CD8^-$ T cells[5].

CD1d-tetramers generated using detergent refolding specifically detected human invariant natural killer (NK)T cells which recognise glycolipid presented by CD1d and show specificity for alpha-galactosylceramide (aGC),(Figure 5). Human NKT cells expressing an invariant TCR Valpha24 chain are highly specific for CD1d/aGC complex. Biotinylated human CD1d molecules loaded with the synthetic glycolipid aGC were generated from completely denatured and reduced CD1d protein and

complexed with fluorecent streptavidin. Fluorescent CD1d/aGC tetramers specifically stained human NKT cells and demonstrated the use of CD1/ligand complexes for *in vivo* and *in vitro* T-cell identification and disease state diagnosis (Figure 5d, e).

Discussion

A unique network of channels allows CD1b to accommodate glycolipids with two very long acyl tails. In CD1b the absence of side chains at Gly98 and Gly116 opens channel T' (Fig 3c sequence alignments). It also indicates that certain of the CD1 family may have the capability to bind three acyl chain lipids. Such ligands would be expected to show strong binding consistent with enhanced avidity. In contrast single acyl chain lipids would be penalized by reduced avidity.

Methods

Protein expression, refolding and crystallization

For expression of human CD1b (hCD1b) in bacterial inclusion bodies the plasmid hCD1b-pET23d, which encodes a truncated form of the hCD1b cDNA containing the extracellular α1-α3 domains, was generated. The hCD1b coding sequence was amplified by PCR from monocyte-derived dendritic cell cDNA. Oligonucleotides used for PCR amplification (5'-3' and 3'-5') introduced 5'Nco1 and 3'BamH1 restriction sites, which allowed cloning into the bacterial expression vector pET23d (Invitrogen). The correct sequence of the hCD1b coding sequence was confirmed using automated sequencing. Plasmid hb2m-pET23d encoding extracellular human beta2-microglobulin (β2m) has been described previously. Both proteins were

expressed separately in E.coli BL21 (Invitrogen) and purified from inclusion bodies as described below.

The extracellular α1- α3 domains of human CD1b (SWISS-PROT: P29016) and β2m were synthesised using a prokaryotic expression system (pET23d; Novagen, Milwaukee, WI). Both proteins were purified from E.coli (strain BL21) inclusion bodies, which were subsequently solubilised using 6M guanidine buffer containing 10mM DTT. Refolding of the fully denatured and reduced proteins was carried out at room temperature by dilution into buffer 1 (1M Urea, 300mM L-Arginine, 50mM Tris pH 7.5, 2mM EDTA, 5mM reduced glutathione, 0.5mM oxidized glutathione) supplemented with 500 μM hexadecyltrimethyl-ammoniumbromide (SIGMA, Illinois, USA) and 1 μM of either synthetic $GM2^{8}$ ligand or soy bean purified PI ligand (AVANTILIPIDS, USA). To remove excess detergent molecules methyl-β-cyclodextrin (FLUKA, Dorset, UK) was added to the refolding mix after 3 days. The refolding mix was concentrated using Amicon stir cells (AMICON, USA) and PM10 membranes (MILLIPORE). The soluble protein fractions were separated from the concentrated refolding mix by size exclusion chromatography using fast liquid pressure chromatography (FPLC; AMERSHAM PHARMACIA, UK) using a Superdex75 16/26 prep grade column (AMERSHAM PHARMACIA) equilibrated with buffer 2 (Tris 20mM, pH 6.0, 30mM NaCl). Monomeric hCD1b/hβ2m-ligand complexes were collected at 150ml elution volume and repurified once in the same buffer. The pure protein peak containing purified monomeric hCD1b/hβ2m-ligand complexes was concentrated at 5mg/ml and used for sitting drop crystallisation[21].

Crystallisation

The best crystals for both complexes hCD1b/hβ2m-GM2 (CD1b/GM2) and hCD1b/hβ2m-PI (CD1b/PI) were grown at 20°C from 2µl of hCD1b protein at 5mg/ml with 1µl of precipitant (0.2M Lithium Nitrate, 20% w/v Polyethylene Glycol 3350, pH 7.1).

Structure Determination

Crystals were flash frozen at 100K in mother liquor containing 20% glycerol. Diffraction data from one CD1b/GM2 crystal were collected at beamline ID-14 EH2 (ESRF, Grenoble France) with 0.933Å radiation, recorded on an ADSC Q4 CCD detector. Diffraction data from two CD1b/PI crystals were collected at beam line ID-29 (ESRF, Grenoble, France) with 0.977Å radiation, recorded on an ADSC Q210 detector.

Processing, merging and reduction of the data were achieved using programs DENZO and SCALEPACK[22]. Processing statistics are given in the Supplementary Information. The crystals belong to space group C2221 (a=87.53Å b=176.89Å c=75.25Å for CD1b/GM2 and a=87.88Å b=177.00Å c=75.28Å for CD1b/PI). In each case, one CD1 molecule per asymmetric unit is present, plus 63% solvent.

The molecular replacement solutions for both the CD1b/GM2 and CD1b/PI crystals were identified with the program AmoRe[23], using respectively, as models, the 2.8Å resolution structure of mCD1d[7] (PDB accession code 1CD1) and the protein component of a partially refined structure of CD1b/GM2. The CNS program suite was used for refinement[24]. Approximately 3% of reflections were set aside for the R_{free} calculations (535 and 751 observations

respectively for the GM2-Cd1b and PI-CD1b structures). The initial rigid body refinement, allowing the α1, α2, α3 and β2m domains to move independently, resulted in an R_{work} of 43.2% (R_{free} of 42.2%) for the CD1b/GM2 and R_{work} of 27.7% (R_{free} of 25.96%) for the CD1b/PI structure. The models were improved through subsequent rebuilding and refinement cycles, which included positional and restrained B factor refinement, geometric regularization, and for the CD1b/PI structure, simulated annealing. The models were rebuilt with the program O[25] into weighted $2F_o-F_c$ and F_o-F_c Φ_{calc} OMIT maps. In the first cycle of the refinement of the GM2-CD1b structure, the murine CD1d β2m sequence was replaced with human CD1b β2m from an HLA-B8 structure (PDB accession code 1AGE). Clear electron density allowed residues in the α3 domain of Cd1d to be mutated to the corresponding residues of CD1b. Further rounds of refinement enabled the rest of the CD1b residues to be located.

Once electron density for segments of acyl chains and individual waters could be identified, for the CD1b/GM2 (R_{work} of 25.4% (R_{free}=30.2%) and for the CD1b/PI (R_{work} of 28.1% (R_{free}=30.2%), these were modelled into the missing density. Atomic models and parameters for the non-glycan portions of the GM2 and PI ligands were obtained from the lipid structure library[26] (http://www.biochem.missouri.edu/~lesa/LIPIDS/membrane_lipid.html). Topology and parameter files for CNS were then produced with the program PRODGM[27] and subsequently edited. Detergent molecules were modelled as alkyl chains.

The final refined structures showed good stereochemistry as assessed with the program PROCHECK[28]. The final model

of CD1b/GM2 has an R_{work} of 22.4% (R_{free}=27.5%) and comprises the CD1b heavy chain (residues A4-A279), the β2m (residues B0-B99), 40 waters and 100 lipid ligand atoms. The final model of CD1b/PI has an R_{work} of 20.3% (R_{free}=23.3%) and comprises the CD1b heavy chain (residues A3-A279), the β2m (residues B0-B99), 232 waters, 3 NO_3 molecules and 90 lipid ligand atoms. VOLUMES (Esnouf, unpublished program) identified cavities as surfaces accessible to methyls (1.7Å radius), but not to large probes (6Å radius). The figures have been prepared using Bobscript[9] and Raster3D[30].

The completeness of the protein and the ligands in the two models increased over the course of the refinement. Comparisons between the GM2-CD1b and PI-CD1b structures furthermore eased the rebuilding procedure of each model. Special care was taken during the refinement to keep the gap between the R_{work} and R_{free} as small as possible, and the R_{free} lower after each refinement cycle.

Generation of fluorescent CD1d tetramers and FACS analysis

Biotinylated human CD1d molecules loaded with the synthetic glycolipid alpha-galactosylceramide (aGC) were generated from completely denatured and reduced inclusion body protein (see Methods - Protein expression, refolding and crystallization). The refolded CD1d molecules were used to generate CD1d/aGC-tetramers by binding the biotinylated CD1d/aGC-complexes to fluorescent streptavidin. The resulting fluorescent CD1d/aGC-tetramers were tested for use as diagnostic compositions in the identification of human invariant NKT cells *in*

vitro by fluorescent cell sorter analysis (FACS). Human invariant NKT cells, known to be highly specific for CD1d/aGC-complex, were stained with FITC-anti-TCR Valpha24 antibody (Figure 5c) and RPE-CD1d/aGC-tetramers (Figure 5d, e). Staining with propidium iodide allowed dead cells to be gated out of the analysis (Figure 5b).

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Table 1

REMARK coordinates from minimization refinement
REMARK refinement resolution: 100 - 2.8 A
REMARK starting r= 0.2241 free_r= 0.2755
REMARK final r= 0.2239 free_r= 0.2751
REMARK rmsd bonds= 0.012288 rmsd angles= 1.72965
REMARK wa= 4.14112
REMARK target= mlf cycles= 1 steps= 200
REMARK sg= C222(1) a= 87.527 b= 176.885 c= 75.250 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1 : CNS_TOPPAR:protein.param
REMARK parameter file 2 : CNS_TOPPAR:water_rep.param
REMARK parameter file 3 : gm2.param
REMARK molecular structure file: water_delete_swt2.mtf
REMARK input coordinates: bindividual_swt2.pdb
REMARK reflection file= smallspot_ren_notrun.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.8
REMARK initial B-factor correction applied to fobs :
REMARK B11= -2.215 B22= 6.610 B33= -4.395
REMARK B12= 0.000 B13= 0.000 B23= 0.000
REMARK B-factor correction applied to coordinate array B: -0.780
REMARK bulk solvent: density level= 0.26028 e/A^3, B-factor= 10 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 14775 (100.0 %)
REMARK number of unobserved reflections (no entry or |F|=0): 1857 (12.6 %)
REMARK number of reflections rejected: 0 (0.0 %)
REMARK total number of reflections used: 12918 (87.4 %)
REMARK number of reflections in working set: 12383 (83.8 %)
REMARK number of reflections in test set: 535 (3.6 %)
CRYST1 87.527 176.885 75.250 90.00 90.00 90.00 C 2 2 21
REMARK FILENAME="/raid1/nathan/cd1/october_ref/minimize2_swt2.pdb"
REMARK DATE:12-Jan-02 23:17:32 created by user: nathan
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ATOM 2 CG PHE A 4 52.914 42.984 -5.978 1.00 80.90 A
ATOM 3 CD1 PHE A 4 53.885 43.591 -5.144 1.00 86.16 A

ATOM 4 CD2 PHE A 4 52.853 41.579 -6.047 1.00 83.50 A
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ATOM 8 C PHE A 4 50.178 43.764 -4.926 1.00 64.77 A
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ATOM 24 O GLY A 6 49.167 38.640 -2.899 1.00 41.42 A
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ATOM 29 CG PRO A 7 48.087 34.621 -4.524 1.00 35.80 A
ATOM 30 C PRO A 7 51.223 36.380 -3.804 1.00 34.41 A
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ATOM 36 CG2 THR A 8 52.712 38.869 -1.784 1.00 37.48 A
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ATOM 41 CB SER A 9 54.350 32.636 -0.578 1.00 33.48 A

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ATOM 243 O ASP A 34 44.794 27.550 -1.944 1.00 29.35 A
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ATOM 250 C LEU A 35 46.473 27.693 -4.976 1.00 23.33 A
ATOM 251 O LEU A 35 47.688 27.894 -5.052 1.00 24.55 A
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ATOM 254 CB GLN A 36 45.846 24.178 -5.860 1.00 18.97 A
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ATOM 256 CD GLN A 36 45.896 21.641 -5.926 1.00 22.38 A
ATOM 257 OE1 GLN A 36 44.738 21.593 -5.485 1.00 25.72 A
ATOM 258 NE2 GLN A 36 46.520 20.573 -6.424 1.00 12.75 A
ATOM 259 C GLN A 36 46.908 25.722 -7.491 1.00 17.93 A
ATOM 260 O GLN A 36 46.011 26.113 -8.234 1.00 22.05 A
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ATOM 262 CA ILE A 37 48.571 25.657 -9.289 1.00 21.88 A
ATOM 263 CB ILE A 37 49.543 26.834 -9.505 1.00 21.23 A
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ATOM 266 CD1 ILE A 37 51.782 27.836 -8.766 1.00 27.96 A
ATOM 267 C ILE A 37 49.161 24.360 -9.833 1.00 26.85 A
ATOM 268 O ILE A 37 49.161 24.134 -11.048 1.00 32.79 A
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ATOM 282 O GLY A 39 50.924 17.980 -9.789 1.00 28.39 A
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ATOM 289 CE3 TRP A 40 54.756 15.904 -9.111 1.00 26.61 A
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ATOM 295 C TRP A 40 50.349 14.230 -8.769 1.00 31.95 A
ATOM 296 O TRP A 40 49.533 13.764 -7.971 1.00 33.56 A
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ATOM 302 OD2 ASP A 41 49.765 9.898 -12.347 1.00 39.63 A
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ATOM 310 O SER A 42 53.586 8.226 -8.614 1.00 49.09 A
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ATOM 474 O VAL A 63 59.912 19.305 -14.653 1.00 52.00 A
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ATOM 479 O ALA A 64 62.377 16.289 -15.200 1.00 42.31 A
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ATOM 544 O ARG A 71 60.803 9.806 -7.039 1.00 37.91 A
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ATOM 546 CA VAL A 72 63.545 10.153 -7.230 1.00 37.24 A
ATOM 547 CB VAL A 72 64.988 10.271 -7.856 1.00 36.44 A
ATOM 548 CG1 VAL A 72 64.945 9.956 -9.347 1.00 33.54 A
ATOM 549 CG2 VAL A 72 65.629 11.631 -7.586 1.00 39.46 A
ATOM 550 C VAL A 72 63.576 10.409 -5.731 1.00 36.23 A
ATOM 551 O VAL A 72 63.908 9.507 -4.961 1.00 43.22 A
ATOM 552 N TYR A 73 63.180 11.625 -5.335 1.00 35.97 A
ATOM 553 CA TYR A 73 63.112 12.039 -3.928 1.00 33.09 A
ATOM 554 CB TYR A 73 62.899 13.563 -3.805 1.00 25.52 A
ATOM 555 CG TYR A 73 62.367 14.060 -2.466 1.00 25.43 A
ATOM 556 CD1 TYR A 73 63.203 14.146 -1.336 1.00 27.77 A
ATOM 557 CE1 TYR A 73 62.692 14.553 -0.068 1.00 30.79 A
ATOM 558 CD2 TYR A 73 61.004 14.399 -2.309 1.00 24.42 A
ATOM 559 CE2 TYR A 73 60.483 14.797 -1.050 1.00 28.72 A
ATOM 560 CZ TYR A 73 61.331 14.869 0.063 1.00 33.24 A
ATOM 561 OH TYR A 73 60.821 15.219 1.292 1.00 32.55 A
ATOM 562 C TYR A 73 61.985 11.279 -3.240 1.00 32.50 A
ATOM 563 O TYR A 73 62.205 10.686 -2.201 1.00 33.75 A
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ATOM 565 CA ILE A 74 59.603 10.627 -3.309 1.00 34.53 A
ATOM 566 CB ILE A 74 58.349 10.954 -4.187 1.00 33.84 A
ATOM 567 CG2 ILE A 74 57.216 9.939 -4.000 1.00 33.36 A
ATOM 568 CG1 ILE A 74 57.869 12.372 -3.845 1.00 30.81 A
ATOM 569 CD1 ILE A 74 56.926 12.992 -4.852 1.00 35.17 A
ATOM 570 C ILE A 74 59.835 9.136 -3.114 1.00 35.24 A
ATOM 571 O ILE A 74 59.363 8.561 -2.133 1.00 40.08 A
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ATOM 577 CD2 PHE A 75 63.182 4.715 -5.346 1.00 39.54 A
ATOM 578 CE1 PHE A 75 61.103 2.799 -5.251 1.00 36.67 A
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ATOM 582 O PHE A 75 61.793 6.181 -1.877 1.00 38.17 A
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ATOM 585 C GLY A 76 63.885 7.944 -0.527 1.00 38.49 A
ATOM 586 O GLY A 76 64.480 7.392 0.390 1.00 35.98 A
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ATOM 602 O ALA A 78 60.686 4.702 2.726 1.00 42.44 A
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ATOM 611 NH2 ARG A 79 68.323 1.666 0.957 1.00 75.56 A

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ATOM 613 O ARG A 79 63.628 2.895 2.881 1.00 51.11 A
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ATOM 640 CA ASP A 83 64.648 1.174 6.215 1.00 50.17 A
ATOM 641 CB ASP A 83 65.789 1.575 5.272 1.00 50.85 A
ATOM 642 CG ASP A 83 66.010 0.587 4.140 1.00 55.35 A
ATOM 643 OD1 ASP A 83 67.003 0.774 3.402 1.00 58.87 A
ATOM 644 OD2 ASP A 83 65.218 -0.370 3.983 1.00 58.34 A
ATOM 645 C ASP A 83 65.096 1.496 7.633 1.00 53.32 A
ATOM 646 O ASP A 83 65.586 0.619 8.347 1.00 53.81 A
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ATOM 666 O GLY A 86 64.082 1.197 15.769 1.00 63.65 A
ATOM 667 N ASP A 87 65.058 1.668 13.772 1.00 60.90 A
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ATOM 669 CB ASP A 87 67.134 2.721 13.069 1.00 65.58 A
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ATOM 672 OD2 ASP A 87 69.022 3.810 14.045 1.00 74.83 A
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ATOM 702 O MET A 90 57.868 2.289 14.550 1.00 66.48 A
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ATOM 721 OH TYR A 92 58.304 1.205 8.496 1.00 48.50 A
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ATOM 723 O TYR A 92 51.338 1.418 13.850 1.00 46.61 A
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ATOM 779 O ILE A 99 58.229 23.106 3.840 1.00 28.65 A
ATOM 780 N ALA A 100 57.596 23.418 1.690 1.00 30.10 A
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ATOM 788 O GLY A 101 60.599 28.593 0.512 1.00 38.68 A
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ATOM 798 CG GLU A 103 57.889 34.552 1.972 1.00 54.77 A
ATOM 799 CD GLU A 103 56.827 34.822 3.028 1.00 60.58 A
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ATOM 801 OE2 GLU A 103 57.018 34.344 4.166 1.00 59.23 A

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ATOM 811 O LEU A 104 56.961 38.822 -0.258 1.00 51.65 A
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ATOM 814 CB HIS A 105 59.670 40.817 1.822 1.00 56.41 A
ATOM 815 CG HIS A 105 59.503 39.648 2.732 1.00 60.07 A
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ATOM 821 O HIS A 105 59.337 42.277 -1.122 1.00 58.96 A
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ATOM 823 CA SER A 106 58.198 44.544 0.015 1.00 56.68 A
ATOM 824 CB SER A 106 57.167 45.463 0.695 1.00 56.74 A
ATOM 825 OG SER A 106 57.282 45.445 2.107 1.00 62.72 A
ATOM 826 C SER A 106 59.636 45.038 0.213 1.00 55.19 A
ATOM 827 O SER A 106 60.214 44.889 1.300 1.00 53.43 A
ATOM 828 N GLY A 107 60.240 45.471 -0.889 1.00 52.61 A
ATOM 829 CA GLY A 107 61.614 45.939 -0.863 1.00 53.14 A
ATOM 830 C GLY A 107 62.495 45.105 -1.778 1.00 51.00 A
ATOM 831 O GLY A 107 63.619 45.510 -2.093 1.00 51.03 A
ATOM 832 N GLY A 108 62.000 43.920 -2.149 1.00 46.61 A
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ATOM 835 O GLY A 108 63.538 40.826 -3.287 1.00 36.01 A
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ATOM 837 CA ALA A 109 63.951 40.427 -0.549 1.00 39.48 A
ATOM 838 CB ALA A 109 64.340 40.733 0.881 1.00 37.77 A
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ATOM 1137 O GLN A 150 77.455 12.941 4.143 1.00 78.99 A
ATOM 1138 N TYR A 151 75.274 13.521 4.261 1.00 79.93 A
ATOM 1139 CA TYR A 151 74.976 13.265 2.852 1.00 80.93 A
ATOM 1140 CB TYR A 151 73.600 12.586 2.713 1.00 82.25 A
ATOM 1141 CG TYR A 151 73.507 11.193 3.318 1.00 86.10 A
ATOM 1142 CD1 TYR A 151 73.788 10.047 2.540 1.00 86.84 A
ATOM 1143 CE1 TYR A 151 73.726 8.740 3.103 1.00 88.91 A

ATOM 1144 CD2 TYR A 151 73.156 11.008 4.675 1.00 86.60 A
ATOM 1145 CE2 TYR A 151 73.091 9.705 5.251 1.00 87.31 A
ATOM 1146 CZ TYR A 151 73.379 8.581 4.455 1.00 89.10 A
ATOM 1147 OH TYR A 151 73.323 7.316 4.995 1.00 91.60 A
ATOM 1148 C TYR A 151 75.014 14.608 2.106 1.00 80.28 A
ATOM 1149 O TYR A 151 73.995 15.293 1.976 1.00 80.47 A
ATOM 1150 N GLN A 152 76.210 14.986 1.648 1.00 79.63 A
ATOM 1151 CA GLN A 152 76.450 16.252 0.937 1.00 77.09 A
ATOM 1152 CB GLN A 152 77.950 16.454 0.696 1.00 79.30 A
ATOM 1153 CG GLN A 152 78.755 16.801 1.931 1.00 78.72 A
ATOM 1154 CD GLN A 152 80.243 16.842 1.645 1.00 80.06 A
ATOM 1155 OE1 GLN A 152 80.748 17.788 1.038 1.00 78.28 A
ATOM 1156 NE2 GLN A 152 80.953 15.806 2.076 1.00 82.01 A
ATOM 1157 C GLN A 152 75.716 16.418 -0.390 1.00 73.74 A
ATOM 1158 O GLN A 152 75.307 17.528 -0.737 1.00 71.09 A
ATOM 1159 N GLY A 153 75.542 15.306 -1.106 1.00 71.65 A
ATOM 1160 CA GLY A 153 74.871 15.308 -2.398 1.00 70.80 A
ATOM 1161 C GLY A 153 73.414 15.737 -2.382 1.00 69.00 A
ATOM 1162 O GLY A 153 72.943 16.354 -3.347 1.00 69.85 A
ATOM 1163 N ILE A 154 72.710 15.423 -1.291 1.00 66.27 A
ATOM 1164 CA ILE A 154 71.302 15.789 -1.152 1.00 62.42 A
ATOM 1165 CB ILE A 154 70.441 14.704 -0.420 1.00 59.44 A
ATOM 1166 CG2 ILE A 154 70.741 13.316 -0.987 1.00 62.29 A
ATOM 1167 CG1 ILE A 154 70.676 14.712 1.088 1.00 61.56 A
ATOM 1168 CD1 ILE A 154 69.637 13.949 1.870 1.00 66.06 A
ATOM 1169 C ILE A 154 71.147 17.151 -0.486 1.00 61.92 A
ATOM 1170 O ILE A 154 70.178 17.857 -0.744 1.00 63.80 A
ATOM 1171 N MET A 155 72.127 17.520 0.339 1.00 60.06 A
ATOM 1172 CA MET A 155 72.132 18.802 1.042 1.00 59.56 A
ATOM 1173 CB MET A 155 73.185 18.796 2.147 1.00 61.15 A
ATOM 1174 CG MET A 155 72.763 18.038 3.393 1.00 63.84 A
ATOM 1175 SD MET A 155 71.413 18.850 4.267 1.00 60.30 A
ATOM 1176 CE MET A 155 72.319 20.221 5.058 1.00 70.78 A
ATOM 1177 C MET A 155 72.388 19.964 0.092 1.00 58.61 A
ATOM 1178 O MET A 155 71.861 21.063 0.284 1.00 56.80 A
ATOM 1179 N GLU A 156 73.177 19.687 -0.947 1.00 58.35 A
ATOM 1180 CA GLU A 156 73.523 20.668 -1.967 1.00 58.69 A
ATOM 1181 CB GLU A 156 74.792 20.225 -2.731 1.00 61.60 A

ATOM 1182 CG GLU A 156 75.244 21.071 -3.957 1.00 65.50 A
ATOM 1183 CD GLU A 156 75.446 22.572 -3.686 1.00 70.83 A
ATOM 1184 OE1 GLU A 156 75.800 22.971 -2.552 1.00 70.53 A
ATOM 1185 OE2 GLU A 156 75.240 23.365 -4.632 1.00 70.43 A
ATOM 1186 C GLU A 156 72.340 20.897 -2.902 1.00 57.35 A
ATOM 1187 O GLU A 156 72.029 22.045 -3.220 1.00 56.91 A
ATOM 1188 N THR A 157 71.645 19.819 -3.275 1.00 55.25 A
ATOM 1189 CA THR A 157 70.486 19.928 -4.164 1.00 55.44 A
ATOM 1190 CB THR A 157 70.111 18.586 -4.836 1.00 56.95 A
ATOM 1191 OG1 THR A 157 70.058 17.546 -3.857 1.00 64.94 A
ATOM 1192 CG2 THR A 157 71.124 18.225 -5.919 1.00 62.42 A
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ATOM 1194 O THR A 157 68.372 21.034 -4.214 1.00 52.87 A
ATOM 1195 N VAL A 158 69.241 20.619 -2.173 1.00 51.61 A
ATOM 1196 CA VAL A 158 68.156 21.256 -1.407 1.00 47.46 A
ATOM 1197 CB VAL A 158 68.064 20.721 0.073 1.00 44.47 A
ATOM 1198 CG1 VAL A 158 67.094 21.557 0.917 1.00 36.48 A
ATOM 1199 CG2 VAL A 158 67.574 19.288 0.084 1.00 39.96 A
ATOM 1200 C VAL A 158 68.463 22.754 -1.398 1.00 48.17 A
ATOM 1201 O VAL A 158 67.567 23.577 -1.589 1.00 48.44 A
ATOM 1202 N ARG A 159 69.751 23.072 -1.245 1.00 49.13 A
ATOM 1203 CA ARG A 159 70.261 24.443 -1.212 1.00 47.29 A
ATOM 1204 CB ARG A 159 71.748 24.438 -0.843 1.00 51.04 A
ATOM 1205 CG ARG A 159 72.224 25.685 -0.109 1.00 56.74 A
ATOM 1206 CD ARG A 159 73.572 26.281 -0.513 1.00 61.94 A
ATOM 1207 NE ARG A 159 73.497 27.050 -1.760 1.00 61.17 A
ATOM 1208 CZ ARG A 159 74.054 26.690 -2.916 1.00 59.53 A
ATOM 1209 NH1 ARG A 159 74.740 25.558 -3.011 1.00 55.39 A
ATOM 1210 NH2 ARG A 159 73.927 27.468 -3.982 1.00 57.15 A
ATOM 1211 C ARG A 159 70.054 25.150 -2.559 1.00 45.64 A
ATOM 1212 O ARG A 159 69.671 26.323 -2.588 1.00 49.41 A
ATOM 1213 N ILE A 160 70.261 24.420 -3.660 1.00 40.09 A
ATOM 1214 CA ILE A 160 70.078 24.956 -5.017 1.00 37.78 A
ATOM 1215 CB ILE A 160 70.593 23.957 -6.122 1.00 38.87 A
ATOM 1216 CG2 ILE A 160 70.258 24.465 -7.544 1.00 34.33 A
ATOM 1217 CG1 ILE A 160 72.109 23.754 -5.992 1.00 36.58 A
ATOM 1218 CD1 ILE A 160 72.666 22.606 -6.832 1.00 39.59 A
ATOM 1219 C ILE A 160 68.588 25.240 -5.229 1.00 36.81 A

ATOM 1220 O ILE A 160 68.212 26.337 -5.645 1.00 36.53 A
ATOM 1221 N LEU A 161 67.756 24.265 -4.868 1.00 34.19 A
ATOM 1222 CA LEU A 161 66.309 24.373 -5.012 1.00 34.58 A
ATOM 1223 CB LEU A 161 65.631 23.061 -4.631 1.00 30.35 A
ATOM 1224 CG LEU A 161 65.611 21.953 -5.681 1.00 33.35 A
ATOM 1225 CD1 LEU A 161 65.130 20.685 -5.017 1.00 36.24 A
ATOM 1226 CD2 LEU A 161 64.733 22.304 -6.870 1.00 35.32 A
ATOM 1227 C LEU A 161 65.671 25.506 -4.222 1.00 36.25 A
ATOM 1228 O LEU A 161 64.927 26.325 -4.767 1.00 34.15 A
ATOM 1229 N LEU A 162 66.064 25.595 -2.960 1.00 36.40 A
ATOM 1230 CA LEU A 162 65.525 26.570 -2.033 1.00 35.92 A
ATOM 1231 CB LEU A 162 65.806 26.069 -0.613 1.00 33.45 A
ATOM 1232 CG LEU A 162 64.813 26.162 0.545 1.00 37.17 A
ATOM 1233 CD1 LEU A 162 63.460 25.613 0.164 1.00 37.61 A
ATOM 1234 CD2 LEU A 162 65.379 25.392 1.734 1.00 35.63 A
ATOM 1235 C LEU A 162 66.016 28.008 -2.198 1.00 36.53 A
ATOM 1236 O LEU A 162 65.215 28.937 -2.162 1.00 34.27 A
ATOM 1237 N TYR A 163 67.309 28.179 -2.465 1.00 38.10 A
ATOM 1238 CA TYR A 163 67.897 29.514 -2.552 1.00 38.58 A
ATOM 1239 CB TYR A 163 69.128 29.582 -1.641 1.00 35.94 A
ATOM 1240 CG TYR A 163 68.826 29.226 -0.187 1.00 37.42 A
ATOM 1241 CD1 TYR A 163 68.187 30.147 0.676 1.00 39.64 A
ATOM 1242 CE1 TYR A 163 67.875 29.801 2.031 1.00 36.87 A
ATOM 1243 CD2 TYR A 163 69.151 27.953 0.329 1.00 31.64 A
ATOM 1244 CE2 TYR A 163 68.846 27.596 1.676 1.00 29.31 A
ATOM 1245 CZ TYR A 163 68.208 28.523 2.512 1.00 34.59 A
ATOM 1246 OH TYR A 163 67.887 28.169 3.801 1.00 34.87 A
ATOM 1247 C TYR A 163 68.191 30.109 -3.925 1.00 40.63 A
ATOM 1248 O TYR A 163 68.460 31.313 -4.035 1.00 40.10 A
ATOM 1249 N GLU A 164 68.116 29.282 -4.967 1.00 42.05 A
ATOM 1250 CA GLU A 164 68.359 29.731 -6.338 1.00 40.86 A
ATOM 1251 CB GLU A 164 69.601 29.058 -6.921 1.00 41.93 A
ATOM 1252 CG GLU A 164 70.915 29.574 -6.355 1.00 51.14 A
ATOM 1253 CD GLU A 164 72.098 28.656 -6.633 1.00 57.70 A
ATOM 1254 OE1 GLU A 164 71.920 27.586 -7.270 1.00 53.58 A
ATOM 1255 OE2 GLU A 164 73.216 29.012 -6.192 1.00 58.25 A
ATOM 1256 C GLU A 164 67.162 29.496 -7.255 1.00 40.66 A
ATOM 1257 O GLU A 164 66.642 30.451 -7.840 1.00 39.05 A

ATOM 1258 N THR A 165 66.695 28.245 -7.322 1.00 39.59 A
ATOM 1259 CA THR A 165 65.571 27.848 -8.180 1.00 40.09 A
ATOM 1260 CB THR A 165 65.483 26.310 -8.320 1.00 38.50 A
ATOM 1261 OG1 THR A 165 66.775 25.797 -8.667 1.00 47.25 A
ATOM 1262 CG2 THR A 165 64.478 25.890 -9.393 1.00 33.05 A
ATOM 1263 C THR A 165 64.216 28.386 -7.741 1.00 41.54 A
ATOM 1264 O THR A 165 63.438 28.841 -8.589 1.00 44.93 A
ATOM 1265 N CYS A 166 63.942 28.355 -6.435 1.00 39.79 A
ATOM 1266 CA CYS A 166 62.663 28.844 -5.912 1.00 38.66 A
ATOM 1267 C CYS A 166 62.429 30.324 -6.236 1.00 37.89 A
ATOM 1268 O CYS A 166 61.351 30.659 -6.734 1.00 37.64 A
ATOM 1269 CB CYS A 166 62.493 28.544 -4.412 1.00 39.64 A
ATOM 1270 SG CYS A 166 60.818 28.826 -3.769 1.00 41.31 A
ATOM 1271 N PRO A 167 63.404 31.228 -5.946 1.00 37.29 A
ATOM 1272 CD PRO A 167 64.592 31.199 -5.066 1.00 35.25 A
ATOM 1273 CA PRO A 167 63.101 32.617 -6.305 1.00 38.07 A
ATOM 1274 CB PRO A 167 64.248 33.400 -5.669 1.00 37.97 A
ATOM 1275 CG PRO A 167 65.322 32.412 -5.484 1.00 39.04 A
ATOM 1276 C PRO A 167 63.023 32.839 -7.815 1.00 39.02 A
ATOM 1277 O PRO A 167 62.153 33.582 -8.277 1.00 41.06 A
ATOM 1278 N ARG A 168 63.834 32.090 -8.575 1.00 37.23 A
ATOM 1279 CA ARG A 168 63.860 32.191 -10.046 1.00 39.91 A
ATOM 1280 CB ARG A 168 64.969 31.308 -10.649 1.00 41.16 A
ATOM 1281 CG ARG A 168 65.219 31.505 -12.155 1.00 40.39 A
ATOM 1282 CD ARG A 168 66.325 30.694 -12.829 1.00 42.32 A
ATOM 1283 NE ARG A 168 66.058 29.252 -12.881 1.00 42.32 A
ATOM 1284 CZ ARG A 168 66.714 28.334 -12.167 1.00 46.28 A
ATOM 1285 NH1 ARG A 168 67.684 28.691 -11.324 1.00 43.53 A
ATOM 1286 NH2 ARG A 168 66.410 27.049 -12.301 1.00 42.08 A
ATOM 1287 C ARG A 168 62.492 31.780 -10.583 1.00 39.46 A
ATOM 1288 O ARG A 168 62.035 32.289 -11.612 1.00 41.98 A
ATOM 1289 N TYR A 169 61.815 30.931 -9.809 1.00 36.29 A
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ATOM 1291 CB TYR A 169 60.213 29.084 -9.538 1.00 27.80 A
ATOM 1292 CG TYR A 169 58.888 28.509 -9.975 1.00 25.28 A
ATOM 1293 CD1 TYR A 169 57.831 28.346 -9.052 1.00 22.28 A
ATOM 1294 CE1 TYR A 169 56.548 27.954 -9.483 1.00 24.86 A
ATOM 1295 CD2 TYR A 169 58.635 28.248 -11.340 1.00 26.87 A

ATOM 1296 CE2 TYR A 169 57.356 27.856 -11.783 1.00 27.00 A
ATOM 1297 CZ TYR A 169 56.323 27.717 -10.852 1.00 26.50 A
ATOM 1298 OH TYR A 169 55.076 27.382 -11.295 1.00 21.85 A
ATOM 1299 C TYR A 169 59.401 31.456 -9.763 1.00 27.58 A
ATOM 1300 O TYR A 169 58.603 31.838 -10.612 1.00 25.33 A
ATOM 1301 N LEU A 170 59.370 31.838 -8.484 1.00 26.90 A
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ATOM 1303 CB LEU A 170 58.832 33.320 -6.575 1.00 24.02 A
ATOM 1304 CG LEU A 170 57.927 33.331 -5.333 1.00 18.56 A
ATOM 1305 CD1 LEU A 170 58.325 34.502 -4.493 1.00 18.70 A
ATOM 1306 CD2 LEU A 170 56.456 33.436 -5.629 1.00 15.04 A
ATOM 1307 C LEU A 170 58.035 33.935 -8.838 1.00 33.55 A
ATOM 1308 O LEU A 170 56.868 34.123 -9.176 1.00 36.23 A
ATOM 1309 N LEU A 171 59.062 34.642 -9.314 1.00 35.21 A
ATOM 1310 CA LEU A 171 58.870 35.797 -10.193 1.00 34.56 A
ATOM 1311 CB LEU A 171 60.181 36.561 -10.406 1.00 36.47 A
ATOM 1312 CG LEU A 171 60.728 37.477 -9.307 1.00 35.71 A
ATOM 1313 CD1 LEU A 171 59.648 38.416 -8.776 1.00 40.31 A
ATOM 1314 CD2 LEU A 171 61.294 36.669 -8.197 1.00 35.90 A
ATOM 1315 C LEU A 171 58.270 35.427 -11.533 1.00 32.95 A
ATOM 1316 O LEU A 171 57.479 36.184 -12.078 1.00 34.00 A
ATOM 1317 N GLY A 172 58.620 34.239 -12.024 1.00 31.81 A
ATOM 1318 CA GLY A 172 58.104 33.751 -13.289 1.00 31.84 A
ATOM 1319 C GLY A 172 56.598 33.550 -13.265 1.00 34.61 A
ATOM 1320 O GLY A 172 55.918 34.023 -14.178 1.00 36.02 A
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ATOM 1322 CA VAL A 173 54.647 32.647 -12.056 1.00 27.68 A
ATOM 1323 CB VAL A 173 54.273 31.540 -11.021 1.00 30.25 A
ATOM 1324 CG1 VAL A 173 53.846 30.276 -11.722 1.00 22.96 A
ATOM 1325 CG2 VAL A 173 55.375 31.299 -10.025 1.00 29.31 A
ATOM 1326 C VAL A 173 53.866 33.863 -11.639 1.00 28.03 A
ATOM 1327 O VAL A 173 52.726 34.016 -12.063 1.00 32.70 A
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ATOM 1329 CA LEU A 174 53.776 35.923 -10.318 1.00 26.44 A
ATOM 1330 CB LEU A 174 54.565 36.628 -9.220 1.00 22.08 A
ATOM 1331 CG LEU A 174 54.622 35.946 -7.849 1.00 26.57 A
ATOM 1332 CD1 LEU A 174 55.348 36.851 -6.885 1.00 22.52 A
ATOM 1333 CD2 LEU A 174 53.245 35.575 -7.301 1.00 29.25 A

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ATOM 1335 O LEU A 174 52.519 37.588 -11.479 1.00 35.07 A
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ATOM 1337 CA ASN A 175 54.382 37.606 -13.634 1.00 29.76 A
ATOM 1338 CB ASN A 175 55.794 37.819 -14.174 1.00 28.17 A
ATOM 1339 CG ASN A 175 55.825 38.705 -15.396 1.00 32.03 A
ATOM 1340 OD1 ASN A 175 56.231 38.266 -16.469 1.00 32.91 A
ATOM 1341 ND2 ASN A 175 55.383 39.955 -15.246 1.00 33.85 A
ATOM 1342 C ASN A 175 53.483 36.947 -14.678 1.00 30.70 A
ATOM 1343 O ASN A 175 52.559 37.585 -15.194 1.00 33.34 A
ATOM 1344 N ALA A 176 53.738 35.667 -14.954 1.00 28.38 A
ATOM 1345 CA ALA A 176 52.964 34.891 -15.929 1.00 26.54 A
ATOM 1346 CB ALA A 176 53.523 33.485 -16.028 1.00 23.51 A
ATOM 1347 C ALA A 176 51.468 34.833 -15.607 1.00 25.36 A
ATOM 1348 O ALA A 176 50.623 34.838 -16.514 1.00 22.95 A
ATOM 1349 N GLY A 177 51.165 34.832 -14.309 1.00 25.53 A
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ATOM 1351 C GLY A 177 49.196 36.079 -13.388 1.00 30.72 A
ATOM 1352 O GLY A 177 48.127 36.073 -12.784 1.00 29.86 A
ATOM 1353 N LYS A 178 49.860 37.188 -13.713 1.00 32.48 A
ATOM 1354 CA LYS A 178 49.427 38.544 -13.360 1.00 35.81 A
ATOM 1355 CB LYS A 178 50.227 39.551 -14.197 1.00 40.27 A
ATOM 1356 CG LYS A 178 50.486 40.898 -13.534 1.00 48.99 A
ATOM 1357 CD LYS A 178 51.037 42.048 -14.393 1.00 59.25 A
ATOM 1358 CE LYS A 178 52.361 41.855 -15.142 1.00 65.20 A
ATOM 1359 NZ LYS A 178 52.230 40.965 -16.336 1.00 63.80 A
ATOM 1360 C LYS A 178 47.916 38.772 -13.580 1.00 35.54 A
ATOM 1361 O LYS A 178 47.225 39.297 -12.700 1.00 32.94 A
ATOM 1362 N ALA A 179 47.417 38.248 -14.706 1.00 34.86 A
ATOM 1363 CA ALA A 179 46.019 38.357 -15.128 1.00 33.38 A
ATOM 1364 CB ALA A 179 45.857 37.756 -16.508 1.00 34.40 A
ATOM 1365 C ALA A 179 44.995 37.750 -14.164 1.00 34.57 A
ATOM 1366 O ALA A 179 43.954 38.358 -13.906 1.00 35.90 A
ATOM 1367 N ASP A 180 45.294 36.563 -13.638 1.00 36.37 A
ATOM 1368 CA ASP A 180 44.413 35.881 -12.689 1.00 36.38 A
ATOM 1369 CB ASP A 180 44.516 34.355 -12.846 1.00 41.17 A
ATOM 1370 CG ASP A 180 43.836 33.826 -14.111 1.00 49.45 A
ATOM 1371 OD1 ASP A 180 43.269 34.627 -14.894 1.00 48.60 A

ATOM 1372 OD2 ASP A 180 43.871 32.587 -14.315 1.00 47.77 A
ATOM 1373 C ASP A 180 44.729 36.251 -11.237 1.00 36.26 A
ATOM 1374 O ASP A 180 43.821 36.458 -10.432 1.00 37.36 A
ATOM 1375 N LEU A 181 46.019 36.357 -10.923 1.00 34.56 A
ATOM 1376 CA LEU A 181 46.495 36.656 -9.573 1.00 34.29 A
ATOM 1377 CB LEU A 181 47.989 36.342 -9.473 1.00 29.14 A
ATOM 1378 CG LEU A 181 48.398 34.875 -9.660 1.00 21.21 A
ATOM 1379 CD1 LEU A 181 49.875 34.778 -9.985 1.00 1.64 A
ATOM 1380 CD2 LEU A 181 48.054 34.063 -8.421 1.00 24.13 A
ATOM 1381 C LEU A 181 46.221 38.054 -9.023 1.00 37.49 A
ATOM 1382 O LEU A 181 45.951 38.205 -7.830 1.00 36.57 A
ATOM 1383 N GLN A 182 46.312 39.070 -9.883 1.00 40.97 A
ATOM 1384 CA GLN A 182 46.078 40.461 -9.479 1.00 41.45 A
ATOM 1385 CB GLN A 182 47.216 41.361 -9.969 1.00 41.13 A
ATOM 1386 CG GLN A 182 48.489 41.201 -9.158 1.00 47.95 A
ATOM 1387 CD GLN A 182 49.672 41.942 -9.741 1.00 52.12 A
ATOM 1388 OE1 GLN A 182 50.648 41.323 -10.173 1.00 53.86 A
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ATOM 1390 C GLN A 182 44.712 40.969 -9.938 1.00 41.79 A
ATOM 1391 O GLN A 182 44.475 42.174 -10.060 1.00 45.06 A
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ATOM 1393 CA ARG A 183 42.420 40.218 -10.531 1.00 40.36 A
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ATOM 1395 CG ARG A 183 40.548 38.788 -11.625 1.00 45.05 A
ATOM 1396 CD ARG A 183 40.040 37.367 -11.786 1.00 49.47 A
ATOM 1397 NE ARG A 183 39.860 36.733 -10.479 1.00 46.56 A
ATOM 1398 CZ ARG A 183 40.178 35.478 -10.183 1.00 50.01 A
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ATOM 1401 C ARG A 183 41.612 40.736 -9.329 1.00 41.17 A
ATOM 1402 O ARG A 183 41.966 40.480 -8.177 1.00 42.90 A
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ATOM 1405 CB GLN A 184 39.898 43.578 -8.445 1.00 37.25 A
ATOM 1406 CG GLN A 184 41.277 44.089 -7.989 1.00 34.78 A
ATOM 1407 CD GLN A 184 41.525 43.969 -6.489 1.00 35.10 A
ATOM 1408 OE1 GLN A 184 42.642 43.689 -6.065 1.00 39.94 A
ATOM 1409 NE2 GLN A 184 40.494 44.191 -5.685 1.00 28.58 A

ATOM 1410 C GLN A 184 38.237 41.716 -8.778 1.00 38.64 A
ATOM 1411 O GLN A 184 37.552 42.412 -9.532 1.00 39.95 A
ATOM 1412 N VAL A 185 37.758 40.637 -8.154 1.00 37.64 A
ATOM 1413 CA VAL A 185 36.362 40.208 -8.283 1.00 32.79 A
ATOM 1414 CB VAL A 185 36.228 38.663 -8.285 1.00 29.14 A
ATOM 1415 CG1 VAL A 185 34.800 38.234 -8.559 1.00 26.50 A
ATOM 1416 CG2 VAL A 185 37.122 38.062 -9.328 1.00 28.22 A
ATOM 1417 C VAL A 185 35.569 40.792 -7.116 1.00 34.54 A
ATOM 1418 O VAL A 185 35.941 40.606 -5.952 1.00 33.29 A
ATOM 1419 N LYS A 186 34.470 41.472 -7.454 1.00 36.12 A
ATOM 1420 CA LYS A 186 33.576 42.129 -6.494 1.00 35.71 A
ATOM 1421 CB LYS A 186 32.707 43.190 -7.200 1.00 42.50 A
ATOM 1422 CG LYS A 186 33.486 44.348 -7.825 1.00 44.32 A
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ATOM 1424 CE LYS A 186 33.491 46.635 -9.060 1.00 49.14 A
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ATOM 1432 CG PRO A 187 32.755 42.324 -2.225 1.00 29.39 A
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ATOM 1446 CB ALA A 189 26.782 41.332 1.044 1.00 36.00 A
ATOM 1447 C ALA A 189 24.785 39.964 0.390 1.00 41.14 A

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ATOM 1723 OE2 GLU A 224 28.249 55.919 8.901 1.00 65.44 A
ATOM 1724 C GLU A 224 29.912 54.317 13.485 1.00 65.29 A
ATOM 1725 O GLU A 224 31.128 54.484 13.611 1.00 68.00 A
ATOM 1726 N GLN A 225 29.178 53.608 14.350 1.00 66.16 A
ATOM 1727 CA GLN A 225 29.746 52.960 15.539 1.00 66.37 A
ATOM 1728 CB GLN A 225 28.978 53.368 16.808 1.00 68.54 A
ATOM 1729 CG GLN A 225 29.544 52.795 18.126 1.00 75.23 A
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ATOM 1732 NE2 GLN A 225 28.687 52.190 20.328 1.00 82.20 A
ATOM 1733 C GLN A 225 29.702 51.444 15.375 1.00 65.18 A
ATOM 1734 O GLN A 225 28.624 50.855 15.314 1.00 67.45 A
ATOM 1735 N GLU A 226 30.879 50.822 15.332 1.00 64.47 A
ATOM 1736 CA GLU A 226 30.994 49.372 15.179 1.00 62.17 A
ATOM 1737 CB GLU A 226 32.310 48.981 14.490 1.00 61.73 A
ATOM 1738 CG GLU A 226 33.563 49.746 14.892 1.00 62.80 A
ATOM 1739 CD GLU A 226 34.715 49.491 13.924 1.00 65.24 A
ATOM 1740 OE1 GLU A 226 35.453 48.502 14.121 1.00 64.30 A
ATOM 1741 OE2 GLU A 226 34.875 50.271 12.955 1.00 63.54 A
ATOM 1742 C GLU A 226 30.793 48.565 16.455 1.00 61.92 A
ATOM 1743 O GLU A 226 31.155 49.006 17.548 1.00 63.35 A
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ATOM 1746 CB GLN A 227 28.679 45.616 17.080 1.00 56.17 A
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ATOM 1804 CB ILE A 235 38.714 33.475 4.849 1.00 42.01 A
ATOM 1805 CG2 ILE A 235 38.537 33.917 3.393 1.00 41.46 A
ATOM 1806 CG1 ILE A 235 38.718 34.741 5.723 1.00 44.63 A
ATOM 1807 CD1 ILE A 235 39.886 35.718 5.462 1.00 52.65 A
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ATOM 1809 O ILE A 235 38.606 30.701 4.079 1.00 41.61 A
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ATOM 1812 CB LEU A 236 34.623 29.049 3.870 1.00 30.03 A
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ATOM 1815 CD2 LEU A 236 35.147 27.988 6.072 1.00 38.34 A
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ATOM 1818 N PRO A 237 36.728 28.614 1.303 1.00 36.06 A
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ATOM 1827 CB ASN A 238 34.194 29.550 -3.835 1.00 46.14 A

ATOM 1828 CG ASN A 238 32.961 29.814 -2.977 1.00 47.61 A
ATOM 1829 OD1 ASN A 238 32.115 28.932 -2.798 1.00 49.02 A
ATOM 1830 ND2 ASN A 238 32.814 31.058 -2.509 1.00 36.72 A
ATOM 1831 C ASN A 238 36.027 27.919 -4.461 1.00 46.92 A
ATOM 1832 O ASN A 238 37.092 28.548 -4.580 1.00 49.25 A
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ATOM 1837 O ALA A 239 37.773 26.912 -8.283 1.00 48.77 A
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ATOM 1849 CG TRP A 241 41.293 30.225 -8.082 1.00 30.24 A
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ATOM 1852 CE3 TRP A 241 43.352 31.574 -8.950 1.00 24.58 A
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ATOM 1859 O TRP A 241 39.128 33.323 -6.327 1.00 27.52 A
ATOM 1860 N THR A 242 37.536 32.028 -5.411 1.00 27.71 A
ATOM 1861 CA THR A 242 36.876 33.119 -4.705 1.00 29.76 A
ATOM 1862 CB THR A 242 35.525 33.509 -5.331 1.00 33.99 A
ATOM 1863 OG1 THR A 242 34.653 32.374 -5.373 1.00 39.34 A
ATOM 1864 CG2 THR A 242 35.708 34.106 -6.735 1.00 35.13 A
ATOM 1865 C THR A 242 36.672 32.695 -3.267 1.00 27.92 A

ATOM 1866 O THR A 242 36.913 31.535 -2.922 1.00 28.80 A
ATOM 1867 N TRP A 243 36.219 33.620 -2.427 1.00 28.54 A
ATOM 1868 CA TRP A 243 36.053 33.318 -1.003 1.00 32.83 A
ATOM 1869 CB TRP A 243 37.063 34.131 -0.189 1.00 33.62 A
ATOM 1870 CG TRP A 243 38.486 33.990 -0.675 1.00 32.25 A
ATOM 1871 CD2 TRP A 243 39.370 32.907 -0.409 1.00 33.41 A
ATOM 1872 CE2 TRP A 243 40.560 33.147 -1.149 1.00 34.43 A
ATOM 1873 CE3 TRP A 243 39.280 31.745 0.384 1.00 36.33 A
ATOM 1874 CD1 TRP A 243 39.152 34.829 -1.528 1.00 33.04 A
ATOM 1875 NE1 TRP A 243 40.396 34.326 -1.823 1.00 34.71 A
ATOM 1876 CZ2 TRP A 243 41.651 32.272 -1.121 1.00 37.63 A
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ATOM 1885 CD1 TYR A 244 30.020 31.847 1.278 1.00 35.33 A
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ATOM 1888 CE2 TYR A 244 29.629 31.193 3.979 1.00 37.18 A
ATOM 1889 CZ TYR A 244 28.522 31.401 3.152 1.00 35.06 A
ATOM 1890 OH TYR A 244 27.249 31.285 3.658 1.00 38.59 A
ATOM 1891 C TYR A 244 33.543 33.466 3.044 1.00 31.88 A
ATOM 1892 O TYR A 244 34.431 32.880 3.668 1.00 31.22 A
ATOM 1893 N LEU A 245 32.783 34.416 3.583 1.00 31.96 A
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ATOM 1895 CB LEU A 245 33.858 36.105 5.029 1.00 32.68 A
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ATOM 1898 CD2 LEU A 245 35.248 37.808 6.215 1.00 35.48 A
ATOM 1899 C LEU A 245 31.597 35.137 5.587 1.00 32.69 A
ATOM 1900 O LEU A 245 30.676 35.624 4.928 1.00 32.92 A
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ATOM 1902 CA ARG A 246 30.301 34.975 7.670 1.00 35.69 A
ATOM 1903 CB ARG A 246 29.908 33.617 8.252 1.00 39.66 A

ATOM 1904 CG ARG A 246 28.467 33.200 8.074 1.00 44.38 A
ATOM 1905 CD ARG A 246 28.077 31.866 8.705 1.00 48.04 A
ATOM 1906 NE ARG A 246 28.544 31.768 10.091 1.00 50.31 A
ATOM 1907 CZ ARG A 246 27.786 31.465 11.143 1.00 48.69 A
ATOM 1908 NH1 ARG A 246 26.488 31.211 11.004 1.00 51.53 A
ATOM 1909 NH2 ARG A 246 28.331 31.459 12.353 1.00 47.77 A
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ATOM 1911 O ARG A 246 31.777 35.879 9.330 1.00 38.57 A
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ATOM 1916 O ALA A 247 27.622 38.205 10.585 1.00 37.24 A
ATOM 1917 N THR A 248 28.754 37.260 12.294 1.00 31.68 A
ATOM 1918 CA THR A 248 27.588 37.163 13.164 1.00 32.17 A
ATOM 1919 CB THR A 248 27.378 35.722 13.669 1.00 32.01 A
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ATOM 1922 C THR A 248 27.542 38.090 14.360 1.00 34.26 A
ATOM 1923 O THR A 248 28.572 38.614 14.789 1.00 35.14 A
ATOM 1924 N LEU A 249 26.323 38.296 14.868 1.00 35.48 A
ATOM 1925 CA LEU A 249 26.062 39.118 16.051 1.00 36.84 A
ATOM 1926 CB LEU A 249 25.761 40.572 15.687 1.00 31.47 A
ATOM 1927 CG LEU A 249 26.460 41.742 16.399 1.00 30.56 A
ATOM 1928 CD1 LEU A 249 25.606 42.967 16.169 1.00 28.95 A
ATOM 1929 CD2 LEU A 249 26.651 41.550 17.896 1.00 33.57 A
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ATOM 1931 O LEU A 249 23.787 38.373 16.266 1.00 39.68 A
ATOM 1932 N ASP A 250 25.109 38.300 18.114 1.00 46.25 A
ATOM 1933 CA ASP A 250 24.080 37.811 19.037 1.00 50.06 A
ATOM 1934 CB ASP A 250 24.714 36.957 20.149 1.00 58.97 A
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ATOM 1936 OD1 ASP A 250 22.483 36.439 20.944 1.00 70.25 A
ATOM 1937 OD2 ASP A 250 24.111 35.059 21.467 1.00 71.83 A
ATOM 1938 C ASP A 250 23.469 39.091 19.616 1.00 48.54 A
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ATOM 1940 N VAL A 251 22.187 39.301 19.332 1.00 47.44 A
ATOM 1941 CA VAL A 251 21.505 40.511 19.771 1.00 50.54 A

ATOM 1942 CB VAL A 251 21.541 41.573 18.604 1.00 47.99 A
ATOM 1943 CG1 VAL A 251 20.314 41.486 17.691 1.00 40.56 A
ATOM 1944 CG2 VAL A 251 21.775 42.965 19.152 1.00 52.67 A
ATOM 1945 C VAL A 251 20.080 40.260 20.280 1.00 52.50 A
ATOM 1946 O VAL A 251 19.480 39.230 19.965 1.00 55.99 A
ATOM 1947 N ALA A 252 19.557 41.211 21.059 1.00 52.52 A
ATOM 1948 CA ALA A 252 18.194 41.145 21.597 1.00 55.64 A
ATOM 1949 CB ALA A 252 18.074 42.024 22.835 1.00 52.54 A
ATOM 1950 C ALA A 252 17.198 41.597 20.512 1.00 57.75 A
ATOM 1951 O ALA A 252 17.557 42.401 19.640 1.00 58.27 A
ATOM 1952 N ASP A 253 15.963 41.087 20.579 1.00 57.26 A
ATOM 1953 CA ASP A 253 14.893 41.383 19.610 1.00 59.25 A
ATOM 1954 CB ASP A 253 13.562 40.813 20.106 1.00 63.27 A
ATOM 1955 CG ASP A 253 13.427 39.323 19.850 1.00 67.20 A
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ATOM 1957 OD2 ASP A 253 12.281 38.863 19.656 1.00 69.35 A
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ATOM 1959 O ASP A 253 14.679 43.097 17.932 1.00 59.76 A
ATOM 1960 N GLY A 254 14.563 43.753 20.098 1.00 58.86 A
ATOM 1961 CA GLY A 254 14.365 45.158 19.778 1.00 59.04 A
ATOM 1962 C GLY A 254 15.591 45.889 19.248 1.00 60.11 A
ATOM 1963 O GLY A 254 15.456 46.859 18.495 1.00 62.17 A
ATOM 1964 N GLU A 255 16.780 45.392 19.597 1.00 59.12 A
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ATOM 1966 CB GLU A 255 19.181 45.508 20.093 1.00 55.52 A
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ATOM 1968 CD GLU A 255 20.188 45.359 22.383 1.00 76.42 A
ATOM 1969 OE1 GLU A 255 20.694 46.225 23.132 1.00 78.97 A
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ATOM 1971 C GLU A 255 18.467 45.744 17.733 1.00 53.87 A
ATOM 1972 O GLU A 255 19.305 46.472 17.197 1.00 52.19 A
ATOM 1973 N ALA A 256 17.865 44.729 17.106 1.00 51.60 A
ATOM 1974 CA ALA A 256 18.146 44.341 15.718 1.00 48.53 A
ATOM 1975 CB ALA A 256 17.327 43.119 15.342 1.00 48.51 A
ATOM 1976 C ALA A 256 17.922 45.454 14.701 1.00 47.66 A
ATOM 1977 O ALA A 256 18.633 45.541 13.700 1.00 48.63 A
ATOM 1978 N ALA A 257 16.958 46.325 14.992 1.00 46.41 A
ATOM 1979 CA ALA A 257 16.638 47.459 14.128 1.00 43.97 A

ATOM 1980 CB ALA A 257 15.263 47.999 14.463 1.00 48.66 A
ATOM 1981 C ALA A 257 17.687 48.544 14.313 1.00 39.32 A
ATOM 1982 O ALA A 257 18.098 48.827 15.438 1.00 37.31 A
ATOM 1983 N GLY A 258 18.130 49.120 13.200 1.00 37.24 A
ATOM 1984 CA GLY A 258 19.141 50.166 13.239 1.00 37.80 A
ATOM 1985 C GLY A 258 20.511 49.617 12.897 1.00 37.65 A
ATOM 1986 O GLY A 258 21.412 50.360 12.484 1.00 36.24 A
ATOM 1987 N LEU A 259 20.656 48.301 13.054 1.00 36.27 A
ATOM 1988 CA LEU A 259 21.906 47.616 12.765 1.00 34.32 A
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ATOM 1990 CG LEU A 259 22.247 46.496 15.065 1.00 30.41 A
ATOM 1991 CD1 LEU A 259 22.090 45.182 15.782 1.00 32.04 A
ATOM 1992 CD2 LEU A 259 23.624 47.080 15.342 1.00 23.96 A
ATOM 1993 C LEU A 259 22.125 47.351 11.283 1.00 34.93 A
ATOM 1994 O LEU A 259 21.181 47.013 10.549 1.00 34.95 A
ATOM 1995 N SER A 260 23.368 47.565 10.852 1.00 32.55 A
ATOM 1996 CA SER A 260 23.768 47.350 9.468 1.00 32.55 A
ATOM 1997 CB SER A 260 23.948 48.678 8.747 1.00 32.20 A
ATOM 1998 OG SER A 260 25.001 49.437 9.312 1.00 39.79 A
ATOM 1999 C SER A 260 25.071 46.585 9.387 1.00 33.59 A
ATOM 2000 O SER A 260 25.849 46.591 10.336 1.00 33.61 A
ATOM 2001 N CYS A 261 25.290 45.913 8.258 1.00 32.32 A
ATOM 2002 CA CYS A 261 26.523 45.164 8.009 1.00 32.30 A
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ATOM 2006 SG CYS A 261 27.733 42.866 6.975 1.00 39.74 A
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ATOM 2015 NH2 ARG A 262 31.577 53.667 5.157 1.00 55.16 A
ATOM 2016 C ARG A 262 30.661 46.016 5.792 1.00 33.30 A
ATOM 2017 O ARG A 262 31.414 45.399 6.550 1.00 37.32 A

ATOM 2018 N VAL A 263 30.789 46.001 4.468 1.00 31.00 A
ATOM 2019 CA VAL A 263 31.818 45.216 3.792 1.00 31.90 A
ATOM 2020 CB VAL A 263 31.191 44.157 2.819 1.00 33.26 A
ATOM 2021 CG1 VAL A 263 32.271 43.310 2.139 1.00 32.38 A
ATOM 2022 CG2 VAL A 263 30.216 43.255 3.555 1.00 35.28 A
ATOM 2023 C VAL A 263 32.764 46.094 2.992 1.00 31.25 A
ATOM 2024 O VAL A 263 32.338 46.769 2.056 1.00 34.55 A
ATOM 2025 N LYS A 264 34.044 46.068 3.362 1.00 32.52 A
ATOM 2026 CA LYS A 264 35.086 46.814 2.652 1.00 32.36 A
ATOM 2027 CB LYS A 264 35.981 47.612 3.603 1.00 34.16 A
ATOM 2028 CG LYS A 264 35.338 48.741 4.383 1.00 36.18 A
ATOM 2029 CD LYS A 264 36.262 49.517 5.323 1.00 33.55 A
ATOM 2030 CE LYS A 264 35.665 50.617 6.182 1.00 35.45 A
ATOM 2031 NZ LYS A 264 35.344 51.834 5.395 1.00 42.44 A
ATOM 2032 C LYS A 264 35.961 45.791 1.940 1.00 32.16 A
ATOM 2033 O LYS A 264 36.399 44.808 2.557 1.00 27.82 A
ATOM 2034 N HIS A 265 36.169 46.008 0.640 1.00 30.87 A
ATOM 2035 CA HIS A 265 37.010 45.144 -0.188 1.00 32.35 A
ATOM 2036 CB HIS A 265 36.191 44.038 -0.867 1.00 33.96 A
ATOM 2037 CG HIS A 265 37.032 43.007 -1.557 1.00 37.88 A
ATOM 2038 CD2 HIS A 265 37.605 41.869 -1.099 1.00 39.55 A
ATOM 2039 ND1 HIS A 265 37.417 43.126 -2.874 1.00 35.97 A
ATOM 2040 CE1 HIS A 265 38.195 42.109 -3.196 1.00 40.43 A
ATOM 2041 NE2 HIS A 265 38.325 41.330 -2.138 1.00 42.02 A
ATOM 2042 C HIS A 265 37.714 46.004 -1.231 1.00 33.27 A
ATOM 2043 O HIS A 265 37.154 46.993 -1.700 1.00 33.48 A
ATOM 2044 N SER A 266 38.927 45.593 -1.602 1.00 34.64 A
ATOM 2045 CA SER A 266 39.774 46.292 -2.574 1.00 37.74 A
ATOM 2046 CB SER A 266 41.129 45.594 -2.657 1.00 37.51 A
ATOM 2047 OG SER A 266 40.969 44.192 -2.779 1.00 44.90 A
ATOM 2048 C SER A 266 39.196 46.492 -3.983 1.00 40.26 A
ATOM 2049 O SER A 266 39.651 47.370 -4.731 1.00 40.94 A
ATOM 2050 N SER A 267 38.193 45.684 -4.329 1.00 41.59 A
ATOM 2051 CA SER A 267 37.525 45.754 -5.634 1.00 43.98 A
ATOM 2052 CB SER A 267 36.990 44.381 -6.028 1.00 45.91 A
ATOM 2053 OG SER A 267 36.049 43.915 -5.079 1.00 49.29 A
ATOM 2054 C SER A 267 36.376 46.746 -5.642 1.00 44.01 A
ATOM 2055 O SER A 267 35.847 47.087 -6.702 1.00 44.88 A

ATOM 2056 N LEU A 268 35.972 47.162 -4.444 1.00 44.95 A
ATOM 2057 CA LEU A 268 34.882 48.110 -4.254 1.00 45.44 A
ATOM 2058 CB LEU A 268 34.246 47.890 -2.880 1.00 38.17 A
ATOM 2059 CG LEU A 268 33.001 46.997 -2.759 1.00 31.97 A
ATOM 2060 CD1 LEU A 268 32.906 45.951 -3.836 1.00 29.01 A
ATOM 2061 CD2 LEU A 268 32.952 46.377 -1.384 1.00 21.26 A
ATOM 2062 C LEU A 268 35.284 49.570 -4.453 1.00 49.67 A
ATOM 2063 O LEU A 268 34.446 50.392 -4.829 1.00 55.61 A
ATOM 2064 N GLU A 269 36.570 49.870 -4.234 1.00 51.59 A
ATOM 2065 CA GLU A 269 37.159 51.213 -4.398 1.00 52.46 A
ATOM 2066 CB GLU A 269 37.346 51.546 -5.890 1.00 54.50 A
ATOM 2067 CG GLU A 269 38.351 50.675 -6.624 1.00 62.03 A
ATOM 2068 CD GLU A 269 38.382 50.965 -8.118 1.00 67.59 A
ATOM 2069 OE1 GLU A 269 37.621 50.316 -8.871 1.00 68.87 A
ATOM 2070 OE2 GLU A 269 39.163 51.846 -8.537 1.00 69.43 A
ATOM 2071 C GLU A 269 36.422 52.355 -3.686 1.00 50.69 A
ATOM 2072 O GLU A 269 35.866 53.256 -4.330 1.00 51.81 A
ATOM 2073 N GLY A 270 36.366 52.259 -2.358 1.00 48.81 A
ATOM 2074 CA GLY A 270 35.712 53.268 -1.543 1.00 48.67 A
ATOM 2075 C GLY A 270 34.211 53.100 -1.417 1.00 51.01 A
ATOM 2076 O GLY A 270 33.632 53.479 -0.394 1.00 51.40 A
ATOM 2077 N GLN A 271 33.587 52.528 -2.453 1.00 51.41 A
ATOM 2078 CA GLN A 271 32.137 52.296 -2.496 1.00 49.20 A
ATOM 2079 CB GLN A 271 31.638 52.245 -3.955 1.00 50.83 A
ATOM 2080 CG GLN A 271 32.080 53.408 -4.864 1.00 61.19 A
ATOM 2081 CD GLN A 271 31.614 54.780 -4.378 1.00 66.33 A
ATOM 2082 OE1 GLN A 271 30.431 55.116 -4.470 1.00 66.77 A
ATOM 2083 NE2 GLN A 271 32.551 55.577 -3.860 1.00 68.10 A
ATOM 2084 C GLN A 271 31.757 51.015 -1.742 1.00 46.36 A
ATOM 2085 O GLN A 271 31.465 49.982 -2.347 1.00 43.32 A
ATOM 2086 N ASP A 272 31.742 51.122 -0.412 1.00 43.62 A
ATOM 2087 CA ASP A 272 31.423 50.023 0.503 1.00 45.65 A
ATOM 2088 CB ASP A 272 31.637 50.463 1.954 1.00 48.57 A
ATOM 2089 CG ASP A 272 33.075 50.831 2.265 1.00 50.79 A
ATOM 2090 OD1 ASP A 272 33.322 51.176 3.443 1.00 48.34 A
ATOM 2091 OD2 ASP A 272 33.950 50.778 1.365 1.00 51.21 A
ATOM 2092 C ASP A 272 30.004 49.483 0.397 1.00 45.62 A
ATOM 2093 O ASP A 272 29.084 50.208 0.015 1.00 51.81 A

ATOM 2094 N ILE A 273 29.838 48.214 0.762 1.00 41.88 A
ATOM 2095 CA ILE A 273 28.538 47.560 0.740 1.00 39.05 A
ATOM 2096 CB ILE A 273 28.656 46.080 0.262 1.00 33.95 A
ATOM 2097 CG2 ILE A 273 27.332 45.325 0.439 1.00 35.02 A
ATOM 2098 CG1 ILE A 273 29.063 46.043 -1.210 1.00 36.23 A
ATOM 2099 CD1 ILE A 273 29.433 44.667 -1.733 1.00 38.45 A
ATOM 2100 C ILE A 273 27.932 47.641 2.143 1.00 40.93 A
ATOM 2101 O ILE A 273 28.441 47.030 3.083 1.00 40.94 A
ATOM 2102 N ILE A 274 26.907 48.483 2.291 1.00 41.06 A
ATOM 2103 CA ILE A 274 26.213 48.620 3.568 1.00 39.84 A
ATOM 2104 CB ILE A 274 26.155 50.079 4.104 1.00 40.69 A
ATOM 2105 CG2 ILE A 274 25.857 50.050 5.594 1.00 45.66 A
ATOM 2106 CG1 ILE A 274 27.510 50.795 3.985 1.00 46.65 A
ATOM 2107 CD1 ILE A 274 27.691 51.628 2.722 1.00 54.78 A
ATOM 2108 C ILE A 274 24.800 48.066 3.374 1.00 40.35 A
ATOM 2109 O ILE A 274 24.092 48.468 2.448 1.00 45.02 A
ATOM 2110 N LEU A 275 24.443 47.085 4.202 1.00 38.45 A
ATOM 2111 CA LEU A 275 23.145 46.411 4.160 1.00 36.48 A
ATOM 2112 CB LEU A 275 23.345 44.949 3.774 1.00 38.10 A
ATOM 2113 CG LEU A 275 22.978 44.441 2.377 1.00 42.93 A
ATOM 2114 CD1 LEU A 275 23.547 45.294 1.247 1.00 42.98 A
ATOM 2115 CD2 LEU A 275 23.471 43.011 2.274 1.00 41.70 A
ATOM 2116 C LEU A 275 22.483 46.495 5.526 1.00 37.90 A
ATOM 2117 O LEU A 275 23.046 46.034 6.515 1.00 42.73 A
ATOM 2118 N TYR A 276 21.265 47.033 5.566 1.00 37.01 A
ATOM 2119 CA TYR A 276 20.528 47.242 6.816 1.00 36.07 A
ATOM 2120 CB TYR A 276 19.879 48.640 6.806 1.00 37.47 A
ATOM 2121 CG TYR A 276 20.827 49.813 6.558 1.00 36.86 A
ATOM 2122 CD1 TYR A 276 21.399 50.034 5.280 1.00 37.88 A
ATOM 2123 CE1 TYR A 276 22.278 51.120 5.038 1.00 38.70 A
ATOM 2124 CD2 TYR A 276 21.155 50.711 7.597 1.00 34.77 A
ATOM 2125 CE2 TYR A 276 22.042 51.804 7.373 1.00 37.81 A
ATOM 2126 CZ TYR A 276 22.597 51.995 6.089 1.00 42.47 A
ATOM 2127 OH TYR A 276 23.479 53.029 5.860 1.00 45.60 A
ATOM 2128 C TYR A 276 19.473 46.184 7.138 1.00 37.59 A
ATOM 2129 O TYR A 276 18.943 45.535 6.239 1.00 37.18 A
ATOM 2130 N TRP A 277 19.148 46.048 8.425 1.00 39.45 A
ATOM 2131 CA TRP A 277 18.150 45.089 8.885 1.00 43.54 A

ATOM 2132 CB TRP A 277 18.412 44.730 10.347 1.00 43.41 A
ATOM 2133 CG TRP A 277 17.714 43.483 10.822 1.00 48.28 A
ATOM 2134 CD2 TRP A 277 18.110 42.120 10.588 1.00 50.56 A
ATOM 2135 CE2 TRP A 277 17.165 41.293 11.256 1.00 52.90 A
ATOM 2136 CE3 TRP A 277 19.172 41.510 9.881 1.00 53.37 A
ATOM 2137 CD1 TRP A 277 16.586 43.426 11.588 1.00 51.70 A
ATOM 2138 NE1 TRP A 277 16.252 42.121 11.853 1.00 55.10 A
ATOM 2139 CZ2 TRP A 277 17.246 39.873 11.243 1.00 52.79 A
ATOM 2140 CZ3 TRP A 277 19.258 40.087 9.865 1.00 54.22 A
ATOM 2141 CH2 TRP A 277 18.292 39.292 10.548 1.00 51.34 A
ATOM 2142 C TRP A 277 16.724 45.626 8.671 1.00 49.68 A
ATOM 2143 O TRP A 277 16.381 46.716 9.131 1.00 47.67 A
ATOM 2144 N ARG A 278 15.913 44.805 8.000 1.00 58.94 A
ATOM 2145 CA ARG A 278 14.520 45.081 7.598 1.00 67.78 A
ATOM 2146 CB ARG A 278 14.017 43.974 6.639 1.00 69.40 A
ATOM 2147 CG ARG A 278 13.807 42.551 7.226 1.00 74.33 A
ATOM 2148 CD ARG A 278 15.009 41.813 7.833 1.00 74.95 A
ATOM 2149 NE ARG A 278 14.770 40.385 8.023 1.00 71.69 A
ATOM 2150 CZ ARG A 278 15.387 39.425 7.337 1.00 70.98 A
ATOM 2151 NH1 ARG A 278 16.287 39.735 6.408 1.00 65.93 A
ATOM 2152 NH2 ARG A 278 15.110 38.149 7.586 1.00 66.80 A
ATOM 2153 C ARG A 278 13.407 45.434 8.597 1.00 72.06 A
ATOM 2154 O ARG A 278 12.565 46.284 8.288 1.00 73.74 A
ATOM 2155 N ASN A 279 13.406 44.792 9.771 1.00 78.01 A
ATOM 2156 CA ASN A 279 12.405 44.968 10.855 1.00 81.98 A
ATOM 2157 CB ASN A 279 12.864 46.002 11.916 1.00 85.12 A
ATOM 2158 CG ASN A 279 13.085 47.406 11.347 1.00 88.76 A
ATOM 2159 OD1 ASN A 279 12.132 48.162 11.122 1.00 85.61 A
ATOM 2160 ND2 ASN A 279 14.348 47.752 11.109 1.00 89.83 A
ATOM 2161 C ASN A 279 10.906 45.145 10.500 1.00 82.59 A
ATOM 2162 O ASN A 279 10.498 46.246 10.059 1.00 82.18 A
ATOM 2163 OXT ASN A 279 10.154 44.156 10.659 1.00 82.60 A
ATOM 2164 CB MET B 0 50.461 8.808 15.966 1.00 72.08 B
ATOM 2165 CG MET B 0 49.619 8.606 14.695 1.00 75.07 B
ATOM 2166 SD MET B 0 47.903 8.083 15.000 1.00 78.58 B
ATOM 2167 CE MET B 0 48.099 6.290 15.077 1.00 77.43 B
ATOM 2168 C MET B 0 49.191 10.659 17.181 1.00 64.97 B
ATOM 2169 O MET B 0 48.575 9.884 17.928 1.00 63.32 B

ATOM 2170 N MET B 0 51.635 10.378 17.503 1.00 68.88 B
ATOM 2171 CA MET B 0 50.516 10.247 16.521 1.00 68.85 B
ATOM 2172 N ILE B 1 48.792 11.905 16.912 1.00 58.77 B
ATOM 2173 CA ILE B 1 47.562 12.492 17.441 1.00 51.80 B
ATOM 2174 CB ILE B 1 47.710 14.028 17.684 1.00 53.80 B
ATOM 2175 CG2 ILE B 1 48.844 14.291 18.648 1.00 57.30 B
ATOM 2176 CG1 ILE B 1 47.941 14.792 16.372 1.00 51.83 B
ATOM 2177 CD1 ILE B 1 47.831 16.304 16.504 1.00 59.34 B
ATOM 2178 C ILE B 1 46.361 12.252 16.530 1.00 48.83 B
ATOM 2179 O ILE B 1 46.518 11.848 15.370 1.00 50.28 B
ATOM 2180 N GLN B 2 45.169 12.505 17.071 1.00 44.89 B
ATOM 2181 CA GLN B 2 43.897 12.352 16.354 1.00 41.39 B
ATOM 2182 CB GLN B 2 43.156 11.092 16.821 1.00 38.74 B
ATOM 2183 CG GLN B 2 43.777 9.761 16.402 1.00 44.87 B
ATOM 2184 CD GLN B 2 43.087 8.549 17.019 1.00 50.26 B
ATOM 2185 OE1 GLN B 2 42.317 8.668 17.981 1.00 47.38 B
ATOM 2186 NE2 GLN B 2 43.371 7.367 16.466 1.00 46.17 B
ATOM 2187 C GLN B 2 43.017 13.577 16.606 1.00 38.06 B
ATOM 2188 O GLN B 2 42.645 13.838 17.749 1.00 39.02 B
ATOM 2189 N ARG B 3 42.736 14.350 15.555 1.00 34.90 B
ATOM 2190 CA ARG B 3 41.886 15.550 15.651 1.00 36.32 B
ATOM 2191 CB ARG B 3 42.619 16.790 15.117 1.00 40.90 B
ATOM 2192 CG ARG B 3 43.905 17.199 15.827 1.00 53.02 B
ATOM 2193 CD ARG B 3 44.827 18.157 15.056 1.00 59.17 B
ATOM 2194 NE ARG B 3 44.915 19.503 15.629 1.00 68.17 B
ATOM 2195 CZ ARG B 3 44.150 20.541 15.283 1.00 70.31 B
ATOM 2196 NH1 ARG B 3 43.206 20.418 14.358 1.00 69.04 B
ATOM 2197 NH2 ARG B 3 44.352 21.725 15.847 1.00 74.08 B
ATOM 2198 C ARG B 3 40.629 15.352 14.805 1.00 33.81 B
ATOM 2199 O ARG B 3 40.729 14.879 13.680 1.00 37.18 B
ATOM 2200 N THR B 4 39.462 15.721 15.334 1.00 33.35 B
ATOM 2201 CA THR B 4 38.179 15.604 14.615 1.00 34.68 B
ATOM 2202 CB THR B 4 36.957 15.633 15.611 1.00 38.39 B
ATOM 2203 OG1 THR B 4 36.907 14.392 16.310 1.00 48.93 B
ATOM 2204 CG2 THR B 4 35.586 15.826 14.901 1.00 35.70 B
ATOM 2205 C THR B 4 38.006 16.728 13.592 1.00 34.78 B
ATOM 2206 O THR B 4 38.385 17.878 13.859 1.00 35.32 B
ATOM 2207 N PRO B 5 37.466 16.403 12.396 1.00 33.78 B

ATOM 2208 CD PRO B 5 37.307 15.071 11.779 1.00 33.19 B
ATOM 2209 CA PRO B 5 37.260 17.439 11.382 1.00 35.70 B
ATOM 2210 CB PRO B 5 36.934 16.626 10.122 1.00 34.88 B
ATOM 2211 CG PRO B 5 36.364 15.362 10.655 1.00 33.48 B
ATOM 2212 C PRO B 5 36.131 18.416 11.712 1.00 35.45 B
ATOM 2213 O PRO B 5 35.123 18.035 12.305 1.00 36.90 B
ATOM 2214 N LYS B 6 36.361 19.686 11.384 1.00 35.90 B
ATOM 2215 CA LYS B 6 35.385 20.755 11.568 1.00 34.66 B
ATOM 2216 CB LYS B 6 36.105 22.094 11.741 1.00 29.82 B
ATOM 2217 CG LYS B 6 35.201 23.253 12.110 1.00 32.98 B
ATOM 2218 CD LYS B 6 35.865 24.596 12.318 1.00 39.98 B
ATOM 2219 CE LYS B 6 34.973 25.767 12.677 1.00 44.26 B
ATOM 2220 NZ LYS B 6 35.773 27.018 12.821 1.00 52.30 B
ATOM 2221 C LYS B 6 34.640 20.713 10.238 1.00 37.33 B
ATOM 2222 O LYS B 6 35.273 20.654 9.179 1.00 41.00 B
ATOM 2223 N ILE B 7 33.311 20.666 10.291 1.00 35.58 B
ATOM 2224 CA ILE B 7 32.501 20.576 9.074 1.00 35.53 B
ATOM 2225 CB ILE B 7 31.628 19.281 9.101 1.00 33.05 B
ATOM 2226 CG2 ILE B 7 30.870 19.099 7.784 1.00 32.20 B
ATOM 2227 CG1 ILE B 7 32.516 18.051 9.326 1.00 36.04 B
ATOM 2228 CD1 ILE B 7 31.835 16.924 10.054 1.00 43.57 B
ATOM 2229 C ILE B 7 31.607 21.793 8.818 1.00 36.85 B
ATOM 2230 O ILE B 7 30.665 22.048 9.570 1.00 40.18 B
ATOM 2231 N GLN B 8 31.886 22.521 7.739 1.00 36.06 B
ATOM 2232 CA GLN B 8 31.071 23.682 7.371 1.00 36.85 B
ATOM 2233 CB GLN B 8 31.907 24.967 7.301 1.00 37.17 B
ATOM 2234 CG GLN B 8 32.150 25.649 8.637 1.00 37.93 B
ATOM 2235 CD GLN B 8 33.625 25.790 8.944 1.00 40.65 B
ATOM 2236 OE1 GLN B 8 34.109 26.892 9.212 1.00 35.89 B
ATOM 2237 NE2 GLN B 8 34.355 24.670 8.901 1.00 43.55 B
ATOM 2238 C GLN B 8 30.362 23.466 6.038 1.00 35.24 B
ATOM 2239 O GLN B 8 31.012 23.205 5.026 1.00 39.48 B
ATOM 2240 N VAL B 9 29.030 23.520 6.051 1.00 31.72 B
ATOM 2241 CA VAL B 9 28.251 23.365 4.825 1.00 27.63 B
ATOM 2242 CB VAL B 9 27.118 22.323 4.941 1.00 24.00 B
ATOM 2243 CG1 VAL B 9 26.559 22.004 3.550 1.00 19.53 B
ATOM 2244 CG2 VAL B 9 27.628 21.058 5.573 1.00 21.81 B
ATOM 2245 C VAL B 9 27.681 24.729 4.458 1.00 29.23 B

ATOM 2246 O VAL B 9 27.085 25.420 5.294 1.00 32.08 B
ATOM 2247 N TYR B 10 27.886 25.109 3.200 1.00 26.34 B
ATOM 2248 CA TYR B 10 27.453 26.403 2.695 1.00 29.29 B
ATOM 2249 CB TYR B 10 28.475 27.485 3.112 1.00 22.81 B
ATOM 2250 CG TYR B 10 29.923 27.211 2.703 1.00 25.25 B
ATOM 2251 CD1 TYR B 10 30.710 26.267 3.399 1.00 28.00 B
ATOM 2252 CE1 TYR B 10 32.042 25.981 3.017 1.00 23.59 B
ATOM 2253 CD2 TYR B 10 30.509 27.878 1.604 1.00 29.82 B
ATOM 2254 CE2 TYR B 10 31.853 27.602 1.211 1.00 31.18 B
ATOM 2255 CZ TYR B 10 32.602 26.649 1.930 1.00 26.91 B
ATOM 2256 OH TYR B 10 33.893 26.371 1.571 1.00 28.91 B
ATOM 2257 C TYR B 10 27.292 26.425 1.176 1.00 34.58 B
ATOM 2258 O TYR B 10 27.959 25.671 0.461 1.00 39.07 B
ATOM 2259 N SER B 11 26.421 27.308 0.689 1.00 35.09 B
ATOM 2260 CA SER B 11 26.214 27.471 -0.744 1.00 35.68 B
ATOM 2261 CB SER B 11 24.733 27.695 -1.077 1.00 39.23 B
ATOM 2262 OG SER B 11 24.172 28.766 -0.336 1.00 40.55 B
ATOM 2263 C SER B 11 27.054 28.664 -1.182 1.00 36.55 B
ATOM 2264 O SER B 11 27.262 29.593 -0.396 1.00 38.35 B
ATOM 2265 N ARG B 12 27.543 28.630 -2.420 1.00 35.87 B
ATOM 2266 CA ARG B 12 28.376 29.704 -2.968 1.00 38.53 B
ATOM 2267 CB ARG B 12 28.956 29.265 -4.325 1.00 38.35 B
ATOM 2268 CG ARG B 12 29.835 30.285 -5.049 1.00 35.25 B
ATOM 2269 CD ARG B 12 30.263 29.961 -6.467 1.00 37.06 B
ATOM 2270 NE ARG B 12 31.071 28.746 -6.544 1.00 37.54 B
ATOM 2271 CZ ARG B 12 31.566 28.242 -7.672 1.00 37.32 B
ATOM 2272 NH1 ARG B 12 31.341 28.838 -8.840 1.00 36.15 B
ATOM 2273 NH2 ARG B 12 32.296 27.135 -7.633 1.00 41.65 B
ATOM 2274 C ARG B 12 27.577 31.003 -3.113 1.00 39.97 B
ATOM 2275 O ARG B 12 28.078 32.087 -2.807 1.00 40.06 B
ATOM 2276 N HIS B 13 26.326 30.860 -3.550 1.00 44.56 B
ATOM 2277 CA HIS B 13 25.401 31.976 -3.780 1.00 46.85 B
ATOM 2278 CB HIS B 13 24.977 31.985 -5.258 1.00 45.38 B
ATOM 2279 CG HIS B 13 26.119 32.124 -6.209 1.00 46.10 B
ATOM 2280 CD2 HIS B 13 26.618 31.272 -7.132 1.00 50.20 B
ATOM 2281 ND1 HIS B 13 26.930 33.236 -6.234 1.00 45.90 B
ATOM 2282 CE1 HIS B 13 27.883 33.062 -7.131 1.00 51.44 B
ATOM 2283 NE2 HIS B 13 27.717 31.877 -7.690 1.00 54.18 B

ATOM 2284 C HIS B 13 24.164 31.806 -2.891 1.00 48.78 B
ATOM 2285 O HIS B 13 23.905 30.696 -2.415 1.00 49.06 B
ATOM 2286 N PRO B 14 23.407 32.903 -2.615 1.00 51.73 B
ATOM 2287 CD PRO B 14 23.684 34.327 -2.898 1.00 52.04 B
ATOM 2288 CA PRO B 14 22.204 32.782 -1.772 1.00 51.62 B
ATOM 2289 CB PRO B 14 21.727 34.229 -1.629 1.00 52.24 B
ATOM 2290 CG PRO B 14 22.328 34.938 -2.816 1.00 56.49 B
ATOM 2291 C PRO B 14 21.120 31.907 -2.384 1.00 52.01 B
ATOM 2292 O PRO B 14 20.871 31.957 -3.596 1.00 54.68 B
ATOM 2293 N ALA B 15 20.494 31.106 -1.529 1.00 52.66 B
ATOM 2294 CA ALA B 15 19.442 30.185 -1.928 1.00 54.66 B
ATOM 2295 CB ALA B 15 19.111 29.253 -0.768 1.00 55.67 B
ATOM 2296 C ALA B 15 18.168 30.845 -2.473 1.00 57.46 B
ATOM 2297 O ALA B 15 17.452 31.553 -1.750 1.00 56.52 B
ATOM 2298 N GLU B 16 17.966 30.666 -3.781 1.00 59.99 B
ATOM 2299 CA GLU B 16 16.796 31.158 -4.507 1.00 62.49 B
ATOM 2300 CB GLU B 16 17.189 32.214 -5.552 1.00 63.82 B
ATOM 2301 CG GLU B 16 15.995 32.929 -6.204 1.00 68.85 B
ATOM 2302 CD GLU B 16 16.385 33.773 -7.407 1.00 71.52 B
ATOM 2303 OE1 GLU B 16 16.609 34.990 -7.241 1.00 71.43 B
ATOM 2304 OE2 GLU B 16 16.458 33.219 -8.526 1.00 76.08 B
ATOM 2305 C GLU B 16 16.255 29.903 -5.192 1.00 63.52 B
ATOM 2306 O GLU B 16 16.888 29.375 -6.114 1.00 65.28 B
ATOM 2307 N ASN B 17 15.104 29.424 -4.711 1.00 64.49 B
ATOM 2308 CA ASN B 17 14.434 28.215 -5.212 1.00 65.95 B
ATOM 2309 CB ASN B 17 13.074 28.044 -4.531 1.00 66.72 B
ATOM 2310 CG ASN B 17 13.176 28.033 -3.016 1.00 70.92 B
ATOM 2311 OD1 ASN B 17 13.077 26.983 -2.379 1.00 70.39 B
ATOM 2312 ND2 ASN B 17 13.378 29.210 -2.430 1.00 71.88 B
ATOM 2313 C ASN B 17 14.267 28.139 -6.734 1.00 68.32 B
ATOM 2314 O ASN B 17 13.711 29.054 -7.356 1.00 68.83 B
ATOM 2315 N GLY B 18 14.827 27.077 -7.319 1.00 68.56 B
ATOM 2316 CA GLY B 18 14.754 26.867 -8.757 1.00 69.41 B
ATOM 2317 C GLY B 18 15.997 27.277 -9.530 1.00 70.05 B
ATOM 2318 O GLY B 18 16.232 26.765 -10.628 1.00 71.16 B
ATOM 2319 N LYS B 19 16.793 28.186 -8.963 1.00 69.27 B
ATOM 2320 CA LYS B 19 18.021 28.668 -9.602 1.00 69.17 B
ATOM 2321 CB LYS B 19 18.301 30.122 -9.193 1.00 69.06 B

ATOM 2322 CG LYS B 19 19.407 30.802 -10.006 1.00 74.59 B
ATOM 2323 CD LYS B 19 19.941 32.141 -9.531 1.00 78.49 B
ATOM 2324 CE LYS B 19 21.151 32.691 -10.280 1.00 79.37 B
ATOM 2325 NZ LYS B 19 21.651 33.975 -9.709 1.00 79.83 B
ATOM 2326 C LYS B 19 19.236 27.785 -9.277 1.00 68.19 B
ATOM 2327 O LYS B 19 19.347 27.262 -8.169 1.00 66.86 B
ATOM 2328 N SER B 20 20.145 27.654 -10.249 1.00 68.73 B
ATOM 2329 CA SER B 20 21.378 26.862 -10.122 1.00 65.77 B
ATOM 2330 CB SER B 20 22.054 26.693 -11.492 1.00 67.03 B
ATOM 2331 OG SER B 20 23.086 25.719 -11.446 1.00 66.71 B
ATOM 2332 C SER B 20 22.335 27.533 -9.136 1.00 63.05 B
ATOM 2333 O SER B 20 22.391 28.764 -9.055 1.00 64.92 B
ATOM 2334 N ASN B 21 23.089 26.709 -8.413 1.00 59.23 B
ATOM 2335 CA ASN B 21 24.023 27.162 -7.379 1.00 55.18 B
ATOM 2336 CB ASN B 21 23.208 27.353 -6.085 1.00 53.71 B
ATOM 2337 CG ASN B 21 23.784 28.392 -5.149 1.00 53.12 B
ATOM 2338 OD1 ASN B 21 24.997 28.569 -5.042 1.00 56.97 B
ATOM 2339 ND2 ASN B 21 22.901 29.078 -4.443 1.00 53.79 B
ATOM 2340 C ASN B 21 25.095 26.072 -7.169 1.00 53.17 B
ATOM 2341 O ASN B 21 25.067 25.037 -7.835 1.00 52.34 B
ATOM 2342 N PHE B 22 26.025 26.311 -6.240 1.00 49.96 B
ATOM 2343 CA PHE B 22 27.098 25.365 -5.894 1.00 46.85 B
ATOM 2344 CB PHE B 22 28.477 25.938 -6.255 1.00 48.09 B
ATOM 2345 CG PHE B 22 28.840 25.809 -7.704 1.00 48.92 B
ATOM 2346 CD1 PHE B 22 29.726 24.792 -8.123 1.00 51.26 B
ATOM 2347 CD2 PHE B 22 28.332 26.715 -8.659 1.00 46.56 B
ATOM 2348 CE1 PHE B 22 30.115 24.671 -9.490 1.00 48.83 B
ATOM 2349 CE2 PHE B 22 28.703 26.614 -10.028 1.00 49.75 B
ATOM 2350 CZ PHE B 22 29.601 25.585 -10.446 1.00 49.54 B
ATOM 2351 C PHE B 22 27.065 25.070 -4.392 1.00 42.99 B
ATOM 2352 O PHE B 22 27.097 26.001 -3.593 1.00 41.26 B
ATOM 2353 N LEU B 23 26.961 23.790 -4.017 1.00 41.76 B
ATOM 2354 CA LEU B 23 26.933 23.370 -2.600 1.00 41.04 B
ATOM 2355 CB LEU B 23 25.997 22.173 -2.383 1.00 43.77 B
ATOM 2356 CG LEU B 23 25.841 21.603 -0.965 1.00 45.20 B
ATOM 2357 CD1 LEU B 23 25.097 22.586 -0.074 1.00 46.74 B
ATOM 2358 CD2 LEU B 23 25.108 20.276 -1.026 1.00 43.33 B
ATOM 2359 C LEU B 23 28.326 22.972 -2.176 1.00 40.16 B

ATOM 2360 O LEU B 23 28.973 22.185 -2.856 1.00 41.82 B
ATOM 2361 N ASN B 24 28.760 23.480 -1.028 1.00 38.02 B
ATOM 2362 CA ASN B 24 30.097 23.197 -0.535 1.00 37.24 B
ATOM 2363 CB ASN B 24 30.944 24.470 -0.522 1.00 37.41 B
ATOM 2364 CG ASN B 24 31.157 25.056 -1.894 1.00 40.13 B
ATOM 2365 OD1 ASN B 24 32.128 24.736 -2.577 1.00 47.35 B
ATOM 2366 ND2 ASN B 24 30.251 25.931 -2.306 1.00 45.19 B
ATOM 2367 C ASN B 24 30.140 22.613 0.857 1.00 37.41 B
ATOM 2368 O ASN B 24 29.317 22.943 1.712 1.00 36.01 B
ATOM 2369 N CYS B 25 31.123 21.742 1.066 1.00 37.06 B
ATOM 2370 CA CYS B 25 31.371 21.135 2.365 1.00 35.95 B
ATOM 2371 C CYS B 25 32.875 21.208 2.587 1.00 36.60 B
ATOM 2372 O CYS B 25 33.655 20.590 1.852 1.00 37.14 B
ATOM 2373 CB CYS B 25 30.900 19.699 2.426 1.00 35.16 B
ATOM 2374 SG CYS B 25 31.080 19.006 4.090 1.00 37.89 B
ATOM 2375 N TYR B 26 33.269 22.015 3.568 1.00 34.57 B
ATOM 2376 CA TYR B 26 34.669 22.219 3.896 1.00 33.81 B
ATOM 2377 CB TYR B 26 34.963 23.719 3.970 1.00 30.30 B
ATOM 2378 CG TYR B 26 36.411 24.104 4.178 1.00 35.29 B
ATOM 2379 CD1 TYR B 26 37.381 23.867 3.179 1.00 38.22 B
ATOM 2380 CE1 TYR B 26 38.735 24.290 3.351 1.00 37.08 B
ATOM 2381 CD2 TYR B 26 36.817 24.764 5.359 1.00 35.96 B
ATOM 2382 CE2 TYR B 26 38.163 25.195 5.542 1.00 33.83 B
ATOM 2383 CZ TYR B 26 39.109 24.954 4.535 1.00 35.97 B
ATOM 2384 OH TYR B 26 40.404 25.382 4.707 1.00 34.85 B
ATOM 2385 C TYR B 26 35.033 21.523 5.198 1.00 34.27 B
ATOM 2386 O TYR B 26 34.568 21.907 6.277 1.00 37.90 B
ATOM 2387 N VAL B 27 35.853 20.483 5.072 1.00 31.15 B
ATOM 2388 CA VAL B 27 36.321 19.717 6.214 1.00 27.96 B
ATOM 2389 CB VAL B 27 36.215 18.188 5.971 1.00 26.79 B
ATOM 2390 CG1 VAL B 27 34.772 17.780 5.976 1.00 30.48 B
ATOM 2391 CG2 VAL B 27 36.829 17.791 4.641 1.00 31.36 B
ATOM 2392 C VAL B 27 37.741 20.153 6.556 1.00 26.22 B
ATOM 2393 O VAL B 27 38.639 20.091 5.715 1.00 25.30 B
ATOM 2394 N SER B 28 37.924 20.621 7.786 1.00 25.41 B
ATOM 2395 CA SER B 28 39.224 21.112 8.243 1.00 27.14 B
ATOM 2396 CB SER B 28 39.282 22.648 8.143 1.00 27.65 B
ATOM 2397 OG SER B 28 38.125 23.259 8.709 1.00 31.43 B

ATOM 2398 C SER B 28 39.589 20.704 9.652 1.00 27.93 B
ATOM 2399 O SER B 28 38.766 20.159 10.391 1.00 22.63 B
ATOM 2400 N GLY B 29 40.844 20.974 10.001 1.00 29.95 B
ATOM 2401 CA GLY B 29 41.358 20.677 11.326 1.00 33.37 B
ATOM 2402 C GLY B 29 41.491 19.219 11.720 1.00 35.23 B
ATOM 2403 O GLY B 29 41.449 18.914 12.912 1.00 40.29 B
ATOM 2404 N PHE B 30 41.643 18.319 10.750 1.00 32.87 B
ATOM 2405 CA PHE B 30 41.771 16.908 11.081 1.00 29.78 B
ATOM 2406 CB PHE B 30 40.762 16.025 10.335 1.00 25.32 B
ATOM 2407 CG PHE B 30 40.826 16.107 8.831 1.00 27.00 B
ATOM 2408 CD1 PHE B 30 40.188 17.155 8.139 1.00 30.39 B
ATOM 2409 CD2 PHE B 30 41.457 15.089 8.086 1.00 25.38 B
ATOM 2410 CE1 PHE B 30 40.169 17.190 6.718 1.00 24.62 B
ATOM 2411 CE2 PHE B 30 41.449 15.107 6.672 1.00 13.54 B
ATOM 2412 CZ PHE B 30 40.802 16.161 5.986 1.00 23.67 B
ATOM 2413 C PHE B 30 43.150 16.350 10.935 1.00 31.26 B
ATOM 2414 O PHE B 30 43.985 16.912 10.238 1.00 33.82 B
ATOM 2415 N HIS B 31 43.361 15.233 11.620 1.00 34.77 B
ATOM 2416 CA HIS B 31 44.612 14.489 11.617 1.00 36.70 B
ATOM 2417 CB HIS B 31 45.662 15.158 12.514 1.00 36.17 B
ATOM 2418 CG HIS B 31 47.053 14.987 12.007 1.00 45.92 B
ATOM 2419 CD2 HIS B 31 47.867 15.836 11.339 1.00 47.61 B
ATOM 2420 ND1 HIS B 31 47.719 13.780 12.060 1.00 55.96 B
ATOM 2421 CE1 HIS B 31 48.878 13.890 11.436 1.00 52.18 B
ATOM 2422 NE2 HIS B 31 48.992 15.128 10.988 1.00 49.25 B
ATOM 2423 C HIS B 31 44.271 13.070 12.114 1.00 37.16 B
ATOM 2424 O HIS B 31 43.574 12.933 13.124 1.00 36.47 B
ATOM 2425 N PRO B 32 44.653 12.003 11.361 1.00 37.20 B
ATOM 2426 CD PRO B 32 44.509 10.669 11.961 1.00 35.64 B
ATOM 2427 CA PRO B 32 45.370 11.869 10.084 1.00 35.18 B
ATOM 2428 CB PRO B 32 45.715 10.381 10.045 1.00 36.59 B
ATOM 2429 CG PRO B 32 45.741 9.991 11.471 1.00 38.22 B
ATOM 2430 C PRO B 32 44.535 12.249 8.871 1.00 35.30 B
ATOM 2431 O PRO B 32 43.350 12.567 9.006 1.00 35.78 B
ATOM 2432 N SER B 33 45.159 12.191 7.697 1.00 34.25 B
ATOM 2433 CA SER B 33 44.519 12.552 6.441 1.00 34.55 B
ATOM 2434 CB SER B 33 45.562 12.667 5.339 1.00 31.04 B
ATOM 2435 OG SER B 33 46.218 11.434 5.124 1.00 41.76 B

ATOM 2436 C SER B 33 43.367 11.676 5.979 1.00 37.63 B
ATOM 2437 O SER B 33 42.342 12.213 5.569 1.00 37.20 B
ATOM 2438 N ASP B 34 43.521 10.349 6.091 1.00 41.78 B
ATOM 2439 CA ASP B 34 42.510 9.348 5.667 1.00 47.23 B
ATOM 2440 CB ASP B 34 42.837 7.957 6.241 1.00 53.47 B
ATOM 2441 CG ASP B 34 44.279 7.534 5.985 1.00 62.66 B
ATOM 2442 OD1 ASP B 34 44.499 6.653 5.128 1.00 67.32 B
ATOM 2443 OD2 ASP B 34 45.193 8.079 6.648 1.00 66.68 B
ATOM 2444 C ASP B 34 41.085 9.746 6.061 1.00 46.20 B
ATOM 2445 O ASP B 34 40.743 9.791 7.246 1.00 49.34 B
ATOM 2446 N ILE B 35 40.301 10.134 5.060 1.00 45.34 B
ATOM 2447 CA ILE B 35 38.932 10.582 5.278 1.00 46.86 B
ATOM 2448 CB ILE B 35 38.918 12.115 5.610 1.00 48.43 B
ATOM 2449 CG2 ILE B 35 39.379 12.929 4.400 1.00 50.45 B
ATOM 2450 CG1 ILE B 35 37.557 12.568 6.158 1.00 48.27 B
ATOM 2451 CD1 ILE B 35 37.565 13.955 6.788 1.00 46.32 B
ATOM 2452 C ILE B 35 38.015 10.267 4.090 1.00 47.42 B
ATOM 2453 O ILE B 35 38.446 10.240 2.928 1.00 50.90 B
ATOM 2454 N GLU B 36 36.749 10.038 4.411 1.00 43.89 B
ATOM 2455 CA GLU B 36 35.726 9.735 3.435 1.00 43.07 B
ATOM 2456 CB GLU B 36 35.248 8.279 3.645 1.00 45.95 B
ATOM 2457 CG GLU B 36 33.851 7.885 3.125 1.00 53.64 B
ATOM 2458 CD GLU B 36 33.677 8.079 1.631 1.00 62.80 B
ATOM 2459 OE1 GLU B 36 34.421 7.442 0.851 1.00 72.82 B
ATOM 2460 OE2 GLU B 36 32.798 8.882 1.247 1.00 58.81 B
ATOM 2461 C GLU B 36 34.619 10.765 3.650 1.00 42.31 B
ATOM 2462 O GLU B 36 34.060 10.868 4.741 1.00 43.22 B
ATOM 2463 N VAL B 37 34.367 11.579 2.627 1.00 39.35 B
ATOM 2464 CA VAL B 37 33.319 12.596 2.691 1.00 38.93 B
ATOM 2465 CB VAL B 37 33.897 14.053 2.679 1.00 39.17 B
ATOM 2466 CG1 VAL B 37 32.783 15.108 2.643 1.00 33.29 B
ATOM 2467 CG2 VAL B 37 34.777 14.302 3.896 1.00 39.65 B
ATOM 2468 C VAL B 37 32.356 12.408 1.522 1.00 40.93 B
ATOM 2469 O VAL B 37 32.771 12.094 0.400 1.00 43.64 B
ATOM 2470 N ASP B 38 31.068 12.576 1.819 1.00 40.80 B
ATOM 2471 CA ASP B 38 29.995 12.465 0.840 1.00 40.50 B
ATOM 2472 CB ASP B 38 29.211 11.164 1.031 1.00 45.22 B
ATOM 2473 CG ASP B 38 29.912 9.968 0.447 1.00 50.50 B

ATOM 2474 OD1 ASP B 38 30.345 10.048 -0.723 1.00 55.61 B
ATOM 2475 OD2 ASP B 38 30.028 8.949 1.160 1.00 53.26 B
ATOM 2476 C ASP B 38 29.027 13.622 0.998 1.00 40.83 B
ATOM 2477 O ASP B 38 28.878 14.181 2.085 1.00 36.47 B
ATOM 2478 N LEU B 39 28.411 14.001 -0.115 1.00 42.61 B
ATOM 2479 CA LEU B 39 27.405 15.052 -0.136 1.00 47.52 B
ATOM 2480 CB LEU B 39 27.692 16.079 -1.238 1.00 47.50 B
ATOM 2481 CG LEU B 39 28.872 17.031 -0.992 1.00 51.72 B
ATOM 2482 CD1 LEU B 39 28.972 18.057 -2.099 1.00 52.77 B
ATOM 2483 CD2 LEU B 39 28.702 17.737 0.334 1.00 49.59 B
ATOM 2484 C LEU B 39 26.089 14.322 -0.375 1.00 52.08 B
ATOM 2485 O LEU B 39 25.968 13.535 -1.318 1.00 53.19 B
ATOM 2486 N LEU B 40 25.139 14.524 0.535 1.00 54.23 B
ATOM 2487 CA LEU B 40 23.848 13.851 0.462 1.00 56.30 B
ATOM 2488 CB LEU B 40 23.467 13.287 1.834 1.00 56.03 B
ATOM 2489 CG LEU B 40 24.497 12.510 2.658 1.00 57.10 B
ATOM 2490 CD1 LEU B 40 23.839 11.958 3.910 1.00 57.03 B
ATOM 2491 CD2 LEU B 40 25.103 11.389 1.838 1.00 53.52 B
ATOM 2492 C LEU B 40 22.701 14.697 -0.047 1.00 59.26 B
ATOM 2493 O LEU B 40 22.702 15.917 0.103 1.00 61.45 B
ATOM 2494 N LYS B 41 21.738 14.020 -0.672 1.00 61.42 B
ATOM 2495 CA LYS B 41 20.522 14.631 -1.195 1.00 59.70 B
ATOM 2496 CB LYS B 41 20.487 14.610 -2.727 1.00 57.93 B
ATOM 2497 CG LYS B 41 19.264 15.289 -3.348 1.00 61.71 B
ATOM 2498 CD LYS B 41 19.149 15.246 -4.871 1.00 67.77 B
ATOM 2499 CE LYS B 41 17.868 15.776 -5.508 1.00 65.67 B
ATOM 2500 NZ LYS B 41 17.644 17.213 -5.209 1.00 68.94 B
ATOM 2501 C LYS B 41 19.421 13.755 -0.627 1.00 60.34 B
ATOM 2502 O LYS B 41 19.236 12.607 -1.056 1.00 59.40 B
ATOM 2503 N ASN B 42 18.764 14.289 0.405 1.00 61.13 B
ATOM 2504 CA ASN B 42 17.656 13.651 1.131 1.00 61.27 B
ATOM 2505 CB ASN B 42 16.399 13.552 0.240 1.00 57.66 B
ATOM 2506 CG ASN B 42 15.987 14.904 -0.350 1.00 59.14 B
ATOM 2507 OD1 ASN B 42 15.671 15.842 0.382 1.00 57.44 B
ATOM 2508 ND2 ASN B 42 16.014 15.008 -1.678 1.00 49.56 B
ATOM 2509 C ASN B 42 18.032 12.298 1.746 1.00 61.22 B
ATOM 2510 O ASN B 42 17.186 11.409 1.888 1.00 65.37 B
ATOM 2511 N GLY B 43 19.311 12.163 2.101 1.00 58.75 B

ATOM 2512 CA GLY B 43 19.817 10.937 2.699 1.00 57.89 B
ATOM 2513 C GLY B 43 20.647 10.050 1.784 1.00 58.41 B
ATOM 2514 O GLY B 43 21.333 9.144 2.266 1.00 55.93 B
ATOM 2515 N GLU B 44 20.583 10.294 0.473 1.00 60.31 B
ATOM 2516 CA GLU B 44 21.338 9.506 -0.508 1.00 63.27 B
ATOM 2517 CB GLU B 44 20.394 8.879 -1.536 1.00 67.99 B
ATOM 2518 CG GLU B 44 19.792 7.558 -1.058 1.00 77.25 B
ATOM 2519 CD GLU B 44 18.479 7.213 -1.732 1.00 83.61 B
ATOM 2520 OE1 GLU B 44 17.521 6.864 -1.002 1.00 84.56 B
ATOM 2521 OE2 GLU B 44 18.403 7.280 -2.982 1.00 87.15 B
ATOM 2522 C GLU B 44 22.448 10.297 -1.192 1.00 62.89 B
ATOM 2523 O GLU B 44 22.242 11.446 -1.595 1.00 60.61 B
ATOM 2524 N ARG B 45 23.611 9.652 -1.337 1.00 62.88 B
ATOM 2525 CA ARG B 45 24.802 10.257 -1.936 1.00 62.14 B
ATOM 2526 CB ARG B 45 26.039 9.367 -1.743 1.00 63.61 B
ATOM 2527 CG ARG B 45 25.951 7.948 -2.302 1.00 74.24 B
ATOM 2528 CD ARG B 45 27.278 7.218 -2.535 1.00 79.20 B
ATOM 2529 NE ARG B 45 28.111 7.909 -3.525 1.00 81.54 B
ATOM 2530 CZ ARG B 45 29.408 8.178 -3.382 1.00 80.45 B
ATOM 2531 NH1 ARG B 45 30.055 7.813 -2.282 1.00 78.77 B
ATOM 2532 NH2 ARG B 45 30.053 8.850 -4.330 1.00 80.03 B
ATOM 2533 C ARG B 45 24.693 10.703 -3.384 1.00 61.36 B
ATOM 2534 O ARG B 45 24.057 10.042 -4.202 1.00 62.25 B
ATOM 2535 N ILE B 46 25.282 11.869 -3.655 1.00 61.33 B
ATOM 2536 CA ILE B 46 25.313 12.491 -4.979 1.00 60.64 B
ATOM 2537 CB ILE B 46 25.397 14.038 -4.845 1.00 57.96 B
ATOM 2538 CG2 ILE B 46 25.365 14.723 -6.229 1.00 58.46 B
ATOM 2539 CG1 ILE B 46 24.231 14.530 -3.979 1.00 56.30 B
ATOM 2540 CD1 ILE B 46 24.303 15.980 -3.544 1.00 53.78 B
ATOM 2541 C ILE B 46 26.509 11.916 -5.757 1.00 63.27 B
ATOM 2542 O ILE B 46 27.598 11.737 -5.198 1.00 60.65 B
ATOM 2543 N GLU B 47 26.291 11.643 -7.044 1.00 65.95 B
ATOM 2544 CA GLU B 47 27.302 11.040 -7.907 1.00 70.55 B
ATOM 2545 CB GLU B 47 26.632 10.412 -9.138 1.00 72.94 B
ATOM 2546 CG GLU B 47 27.251 9.080 -9.585 1.00 75.80 B
ATOM 2547 CD GLU B 47 27.129 7.978 -8.534 1.00 76.24 B
ATOM 2548 OE1 GLU B 47 26.047 7.355 -8.456 1.00 78.44 B
ATOM 2549 OE2 GLU B 47 28.109 7.739 -7.791 1.00 74.16 B

ATOM 2550 C GLU B 47 28.510 11.889 -8.315 1.00 72.59 B
ATOM 2551 O GLU B 47 29.648 11.544 -7.967 1.00 74.59 B
ATOM 2552 N LYS B 48 28.271 12.969 -9.062 1.00 72.15 B
ATOM 2553 CA LYS B 48 29.352 13.849 -9.515 1.00 70.12 B
ATOM 2554 CB LYS B 48 29.014 14.490 -10.872 1.00 72.79 B
ATOM 2555 CG LYS B 48 29.311 13.632 -12.109 1.00 78.25 B
ATOM 2556 CD LYS B 48 28.420 12.425 -12.398 1.00 83.12 B
ATOM 2557 CE LYS B 48 28.547 11.774 -13.771 1.00 84.55 B
ATOM 2558 NZ LYS B 48 29.916 11.243 -14.034 1.00 85.11 B
ATOM 2559 C LYS B 48 29.697 14.924 -8.481 1.00 66.85 B
ATOM 2560 O LYS B 48 29.023 15.958 -8.385 1.00 66.94 B
ATOM 2561 N VAL B 49 30.706 14.624 -7.661 1.00 60.19 B
ATOM 2562 CA VAL B 49 31.192 15.530 -6.615 1.00 54.61 B
ATOM 2563 CB VAL B 49 30.930 14.965 -5.173 1.00 56.47 B
ATOM 2564 CG1 VAL B 49 31.430 15.941 -4.114 1.00 56.12 B
ATOM 2565 CG2 VAL B 49 29.455 14.666 -4.946 1.00 54.06 B
ATOM 2566 C VAL B 49 32.702 15.675 -6.784 1.00 50.10 B
ATOM 2567 O VAL B 49 33.431 14.687 -6.676 1.00 52.15 B
ATOM 2568 N GLU B 50 33.173 16.891 -7.043 1.00 44.78 B
ATOM 2569 CA GLU B 50 34.612 17.110 -7.184 1.00 43.51 B
ATOM 2570 CB GLU B 50 34.936 18.188 -8.218 1.00 48.25 B
ATOM 2571 CG GLU B 50 34.594 17.859 -9.658 1.00 57.23 B
ATOM 2572 CD GLU B 50 33.228 18.380 -10.063 1.00 66.14 B
ATOM 2573 OE1 GLU B 50 32.326 17.544 -10.306 1.00 72.78 B
ATOM 2574 OE2 GLU B 50 33.058 19.623 -10.134 1.00 62.71 B
ATOM 2575 C GLU B 50 35.206 17.506 -5.841 1.00 38.99 B
ATOM 2576 O GLU B 50 34.489 17.988 -4.955 1.00 37.62 B
ATOM 2577 N HIS B 51 36.501 17.254 -5.677 1.00 33.63 B
ATOM 2578 CA HIS B 51 37.196 17.605 -4.443 1.00 30.83 B
ATOM 2579 CB HIS B 51 37.145 16.469 -3.405 1.00 32.98 B
ATOM 2580 CG HIS B 51 37.798 15.188 -3.841 1.00 41.75 B
ATOM 2581 CD2 HIS B 51 39.008 14.656 -3.541 1.00 45.53 B
ATOM 2582 ND1 HIS B 51 37.193 14.298 -4.702 1.00 47.24 B
ATOM 2583 CE1 HIS B 51 38.003 13.276 -4.918 1.00 48.79 B
ATOM 2584 NE2 HIS B 51 39.112 13.469 -4.225 1.00 47.55 B
ATOM 2585 C HIS B 51 38.625 18.036 -4.676 1.00 28.11 B
ATOM 2586 O HIS B 51 39.323 17.470 -5.523 1.00 32.23 B
ATOM 2587 N SER B 52 39.075 18.995 -3.872 1.00 24.01 B

ATOM 2588 CA SER B 52 40.442 19.504 -3.956 1.00 22.58 B
ATOM 2589 CB SER B 52 40.607 20.691 -3.011 1.00 23.84 B
ATOM 2590 OG SER B 52 40.312 20.321 -1.673 1.00 23.68 B
ATOM 2591 C SER B 52 41.459 18.431 -3.565 1.00 22.93 B
ATOM 2592 O SER B 52 41.122 17.457 -2.865 1.00 21.70 B
ATOM 2593 N ASP B 53 42.700 18.601 -4.023 1.00 20.78 B
ATOM 2594 CA ASP B 53 43.767 17.663 -3.665 1.00 19.44 B
ATOM 2595 CB ASP B 53 45.037 17.893 -4.490 1.00 15.16 B
ATOM 2596 CG ASP B 53 44.881 17.492 -5.943 1.00 13.07 B
ATOM 2597 OD1 ASP B 53 43.895 16.812 -6.305 1.00 22.42 B
ATOM 2598 OD2 ASP B 53 45.763 17.860 -6.737 1.00 17.12 B
ATOM 2599 C ASP B 53 44.053 17.943 -2.202 1.00 20.25 B
ATOM 2600 O ASP B 53 43.672 19.006 -1.681 1.00 16.31 B
ATOM 2601 N LEU B 54 44.697 16.990 -1.535 1.00 23.25 B
ATOM 2602 CA LEU B 54 45.004 17.131 -0.119 1.00 21.92 B
ATOM 2603 CB LEU B 54 45.663 15.867 0.438 1.00 22.71 B
ATOM 2604 CG LEU B 54 45.911 15.831 1.954 1.00 19.17 B
ATOM 2605 CD1 LEU B 54 44.607 15.764 2.745 1.00 15.53 B
ATOM 2606 CD2 LEU B 54 46.765 14.651 2.260 1.00 21.11 B
ATOM 2607 C LEU B 54 45.869 18.331 0.181 1.00 23.12 B
ATOM 2608 O LEU B 54 46.822 18.631 -0.544 1.00 24.88 B
ATOM 2609 N SER B 55 45.470 19.041 1.228 1.00 22.11 B
ATOM 2610 CA SER B 55 46.189 20.203 1.682 1.00 22.03 B
ATOM 2611 CB SER B 55 45.557 21.445 1.101 1.00 24.87 B
ATOM 2612 OG SER B 55 46.416 22.570 1.226 1.00 18.26 B
ATOM 2613 C SER B 55 46.160 20.280 3.190 1.00 22.62 B
ATOM 2614 O SER B 55 45.372 19.589 3.848 1.00 23.89 B
ATOM 2615 N PHE B 56 47.065 21.086 3.730 1.00 20.60 B
ATOM 2616 CA PHE B 56 47.136 21.315 5.163 1.00 23.11 B
ATOM 2617 CB PHE B 56 48.036 20.292 5.893 1.00 15.39 B
ATOM 2618 CG PHE B 56 49.422 20.175 5.348 1.00 12.76 B
ATOM 2619 CD1 PHE B 56 49.767 19.075 4.550 1.00 9.42 B
ATOM 2620 CD2 PHE B 56 50.409 21.133 5.668 1.00 4.77 B
ATOM 2621 CE1 PHE B 56 51.080 18.915 4.074 1.00 10.26 B
ATOM 2622 CE2 PHE B 56 51.720 20.996 5.201 1.00 12.21 B
ATOM 2623 CZ PHE B 56 52.066 19.880 4.401 1.00 15.61 B
ATOM 2624 C PHE B 56 47.508 22.760 5.493 1.00 25.39 B
ATOM 2625 O PHE B 56 48.205 23.440 4.715 1.00 25.47 B

ATOM 2626 N SER B 57 47.005 23.224 6.633 1.00 25.41 B
ATOM 2627 CA SER B 57 47.265 24.572 7.116 1.00 27.42 B
ATOM 2628 CB SER B 57 46.086 25.036 7.977 1.00 26.25 B
ATOM 2629 OG SER B 57 45.765 24.067 8.958 1.00 27.53 B
ATOM 2630 C SER B 57 48.590 24.616 7.898 1.00 28.95 B
ATOM 2631 O SER B 57 49.280 23.599 8.013 1.00 27.75 B
ATOM 2632 N LYS B 58 48.929 25.792 8.426 1.00 34.97 B
ATOM 2633 CA LYS B 58 50.162 26.029 9.191 1.00 40.62 B
ATOM 2634 CB LYS B 58 50.181 27.466 9.722 1.00 46.52 B
ATOM 2635 CG LYS B 58 51.163 28.409 9.020 1.00 56.78 B
ATOM 2636 CD LYS B 58 52.677 28.151 9.168 1.00 64.53 B
ATOM 2637 CE LYS B 58 53.304 28.121 10.571 1.00 65.62 B
ATOM 2638 NZ LYS B 58 53.145 29.402 11.320 1.00 68.67 B
ATOM 2639 C LYS B 58 50.432 25.066 10.351 1.00 41.74 B
ATOM 2640 O LYS B 58 51.522 24.486 10.440 1.00 41.58 B
ATOM 2641 N ASP B 59 49.410 24.849 11.182 1.00 41.20 B
ATOM 2642 CA ASP B 59 49.493 23.962 12.350 1.00 39.21 B
ATOM 2643 CB ASP B 59 48.375 24.300 13.354 1.00 44.59 B
ATOM 2644 CG ASP B 59 46.974 24.109 12.778 1.00 49.63 B
ATOM 2645 OD1 ASP B 59 46.618 24.815 11.806 1.00 57.41 B
ATOM 2646 OD2 ASP B 59 46.235 23.252 13.305 1.00 49.33 B
ATOM 2647 C ASP B 59 49.483 22.469 12.002 1.00 36.58 B
ATOM 2648 O ASP B 59 49.325 21.616 12.884 1.00 38.70 B
ATOM 2649 N TRP B 60 49.708 22.183 10.713 1.00 32.93 B
ATOM 2650 CA TRP B 60 49.765 20.839 10.100 1.00 27.57 B
ATOM 2651 CB TRP B 60 50.847 19.951 10.734 1.00 27.06 B
ATOM 2652 CG TRP B 60 52.198 20.578 10.843 1.00 34.72 B
ATOM 2653 CD2 TRP B 60 53.167 20.716 9.803 1.00 31.34 B
ATOM 2654 CE2 TRP B 60 54.315 21.313 10.382 1.00 32.06 B
ATOM 2655 CE3 TRP B 60 53.189 20.382 8.437 1.00 35.14 B
ATOM 2656 CD1 TRP B 60 52.771 21.091 11.975 1.00 34.54 B
ATOM 2657 NE1 TRP B 60 54.041 21.530 11.706 1.00 38.12 B
ATOM 2658 CZ2 TRP B 60 55.480 21.586 9.641 1.00 36.70 B
ATOM 2659 CZ3 TRP B 60 54.357 20.650 7.691 1.00 39.62 B
ATOM 2660 CH2 TRP B 60 55.483 21.247 8.303 1.00 35.76 B
ATOM 2661 C TRP B 60 48.469 20.046 9.995 1.00 24.18 B
ATOM 2662 O TRP B 60 48.483 18.904 9.546 1.00 22.06 B
ATOM 2663 N SER B 61 47.346 20.642 10.386 1.00 24.38 B

ATOM 2664 CA SER B 61 46.065 19.945 10.299 1.00 23.79 B
ATOM 2665 CB SER B 61 45.038 20.567 11.244 1.00 19.91 B
ATOM 2666 OG SER B 61 44.529 21.796 10.751 1.00 25.95 B
ATOM 2667 C SER B 61 45.577 19.984 8.854 1.00 22.56 B
ATOM 2668 O SER B 61 45.799 20.967 8.145 1.00 22.63 B
ATOM 2669 N PHE B 62 44.914 18.917 8.429 1.00 23.59 B
ATOM 2670 CA PHE B 62 44.419 18.804 7.059 1.00 23.93 B
ATOM 2671 CB PHE B 62 44.355 17.342 6.643 1.00 18.06 B
ATOM 2672 CG PHE B 62 45.651 16.619 6.778 1.00 19.45 B
ATOM 2673 CD1 PHE B 62 46.600 16.662 5.748 1.00 23.94 B
ATOM 2674 CD2 PHE B 62 45.925 15.857 7.920 1.00 21.34 B
ATOM 2675 CE1 PHE B 62 47.813 15.946 5.845 1.00 21.53 B
ATOM 2676 CE2 PHE B 62 47.137 15.132 8.035 1.00 24.47 B
ATOM 2677 CZ PHE B 62 48.080 15.175 6.993 1.00 19.80 B
ATOM 2678 C PHE B 62 43.079 19.458 6.767 1.00 27.06 B
ATOM 2679 O PHE B 62 42.219 19.566 7.655 1.00 28.41 B
ATOM 2680 N TYR B 63 42.920 19.896 5.515 1.00 26.79 B
ATOM 2681 CA TYR B 63 41.683 20.520 5.050 1.00 23.29 B
ATOM 2682 CB TYR B 63 41.720 22.054 5.209 1.00 13.04 B
ATOM 2683 CG TYR B 63 42.595 22.824 4.250 1.00 15.86 B
ATOM 2684 CD1 TYR B 63 42.112 23.215 2.976 1.00 13.19 B
ATOM 2685 CE1 TYR B 63 42.894 23.982 2.091 1.00 15.30 B
ATOM 2686 CD2 TYR B 63 43.886 23.217 4.615 1.00 16.66 B
ATOM 2687 CE2 TYR B 63 44.689 23.999 3.727 1.00 21.33 B
ATOM 2688 CZ TYR B 63 44.176 24.372 2.472 1.00 19.35 B
ATOM 2689 OH TYR B 63 44.933 25.116 1.599 1.00 31.88 B
ATOM 2690 C TYR B 63 41.346 20.100 3.622 1.00 23.29 B
ATOM 2691 O TYR B 63 42.251 19.877 2.813 1.00 25.58 B
ATOM 2692 N LEU B 64 40.051 20.007 3.315 1.00 22.03 B
ATOM 2693 CA LEU B 64 39.563 19.618 1.978 1.00 21.65 B
ATOM 2694 CB LEU B 64 39.394 18.093 1.867 1.00 14.45 B
ATOM 2695 CG LEU B 64 40.589 17.158 1.699 1.00 18.34 B
ATOM 2696 CD1 LEU B 64 40.201 15.752 2.073 1.00 18.41 B
ATOM 2697 CD2 LEU B 64 41.124 17.236 0.284 1.00 22.35 B
ATOM 2698 C LEU B 64 38.210 20.257 1.673 1.00 22.35 B
ATOM 2699 O LEU B 64 37.387 20.456 2.577 1.00 22.45 B
ATOM 2700 N LEU B 65 37.971 20.532 0.393 1.00 18.35 B
ATOM 2701 CA LEU B 65 36.716 21.124 -0.052 1.00 21.33 B

ATOM 2702 CB LEU B 65 36.964 22.482 -0.732 1.00 21.01 B
ATOM 2703 CG LEU B 65 35.784 23.240 -1.381 1.00 24.09 B
ATOM 2704 CD1 LEU B 65 34.841 23.788 -0.329 1.00 20.98 B
ATOM 2705 CD2 LEU B 65 36.294 24.369 -2.262 1.00 27.19 B
ATOM 2706 C LEU B 65 36.015 20.178 -1.020 1.00 23.30 B
ATOM 2707 O LEU B 65 36.616 19.714 -1.989 1.00 28.77 B
ATOM 2708 N TYR B 66 34.752 19.882 -0.730 1.00 24.64 B
ATOM 2709 CA TYR B 66 33.923 19.013 -1.567 1.00 28.50 B
ATOM 2710 CB TYR B 66 33.388 17.816 -0.757 1.00 27.32 B
ATOM 2711 CG TYR B 66 34.387 16.678 -0.579 1.00 29.42 B
ATOM 2712 CD1 TYR B 66 35.538 16.835 0.226 1.00 32.05 B
ATOM 2713 CE1 TYR B 66 36.503 15.789 0.359 1.00 36.28 B
ATOM 2714 CD2 TYR B 66 34.208 15.446 -1.245 1.00 27.32 B
ATOM 2715 CE2 TYR B 66 35.163 14.388 -1.122 1.00 33.06 B
ATOM 2716 CZ TYR B 66 36.307 14.577 -0.322 1.00 37.59 B
ATOM 2717 OH TYR B 66 37.264 13.593 -0.234 1.00 42.84 B
ATOM 2718 C TYR B 66 32.780 19.881 -2.088 1.00 30.24 B
ATOM 2719 O TYR B 66 32.093 20.542 -1.298 1.00 30.40 B
ATOM 2720 N TYR B 67 32.607 19.899 -3.412 1.00 28.39 B
ATOM 2721 CA TYR B 67 31.582 20.713 -4.057 1.00 32.55 B
ATOM 2722 CB TYR B 67 32.190 22.056 -4.530 1.00 31.23 B
ATOM 2723 CG TYR B 67 33.308 21.958 -5.564 1.00 30.03 B
ATOM 2724 CD1 TYR B 67 34.618 21.578 -5.190 1.00 28.84 B
ATOM 2725 CE1 TYR B 67 35.659 21.449 -6.154 1.00 35.20 B
ATOM 2726 CD2 TYR B 67 33.054 22.219 -6.926 1.00 31.93 B
ATOM 2727 CE2 TYR B 67 34.087 22.097 -7.911 1.00 39.48 B
ATOM 2728 CZ TYR B 67 35.385 21.712 -7.514 1.00 40.91 B
ATOM 2729 OH TYR B 67 36.386 21.600 -8.460 1.00 41.41 B
ATOM 2730 C TYR B 67 30.844 20.037 -5.215 1.00 38.26 B
ATOM 2731 O TYR B 67 31.322 19.036 -5.758 1.00 43.29 B
ATOM 2732 N THR B 68 29.703 20.627 -5.599 1.00 42.22 B
ATOM 2733 CA THR B 68 28.846 20.167 -6.708 1.00 44.75 B
ATOM 2734 CB THR B 68 28.070 18.838 -6.374 1.00 46.21 B
ATOM 2735 OG1 THR B 68 27.339 18.408 -7.529 1.00 49.56 B
ATOM 2736 CG2 THR B 68 27.106 19.010 -5.201 1.00 40.47 B
ATOM 2737 C THR B 68 27.840 21.245 -7.140 1.00 46.84 B
ATOM 2738 O THR B 68 27.291 21.955 -6.285 1.00 42.69 B
ATOM 2739 N GLU B 69 27.587 21.323 -8.456 1.00 48.87 B

ATOM 2740 CA GLU B 69 26.644 22.282 -9.062 1.00 51.22 B
ATOM 2741 CB GLU B 69 26.985 22.520 -10.551 1.00 50.00 B
ATOM 2742 CG GLU B 69 26.182 23.654 -11.226 1.00 57.19 B
ATOM 2743 CD GLU B 69 26.479 23.816 -12.716 1.00 63.28 B
ATOM 2744 OE1 GLU B 69 27.480 24.484 -13.057 1.00 65.49 B
ATOM 2745 OE2 GLU B 69 25.698 23.296 -13.550 1.00 65.09 B
ATOM 2746 C GLU B 69 25.198 21.781 -8.912 1.00 52.54 B
ATOM 2747 O GLU B 69 24.726 20.981 -9.721 1.00 52.73 B
ATOM 2748 N PHE B 70 24.495 22.287 -7.897 1.00 55.19 B
ATOM 2749 CA PHE B 70 23.120 21.867 -7.621 1.00 58.77 B
ATOM 2750 CB PHE B 70 23.023 21.303 -6.179 1.00 60.76 B
ATOM 2751 CG PHE B 70 22.885 22.350 -5.075 1.00 60.87 B
ATOM 2752 CD1 PHE B 70 23.673 23.516 -5.037 1.00 61.60 B
ATOM 2753 CD2 PHE B 70 21.946 22.155 -4.055 1.00 63.40 B
ATOM 2754 CE1 PHE B 70 23.516 24.475 -3.991 1.00 61.44 B
ATOM 2755 CE2 PHE B 70 21.779 23.101 -3.002 1.00 63.67 B
ATOM 2756 CZ PHE B 70 22.569 24.264 -2.974 1.00 61.27 B
ATOM 2757 C PHE B 70 22.021 22.899 -7.903 1.00 60.56 B
ATOM 2758 O PHE B 70 22.312 24.056 -8.199 1.00 60.13 B
ATOM 2759 N THR B 71 20.768 22.465 -7.760 1.00 62.83 B
ATOM 2760 CA THR B 71 19.592 23.309 -7.967 1.00 65.10 B
ATOM 2761 CB THR B 71 18.885 22.962 -9.309 1.00 63.04 B
ATOM 2762 OG1 THR B 71 19.829 23.084 -10.380 1.00 63.34 B
ATOM 2763 CG2 THR B 71 17.712 23.909 -9.582 1.00 62.09 B
ATOM 2764 C THR B 71 18.645 23.127 -6.761 1.00 67.09 B
ATOM 2765 O THR B 71 17.950 22.110 -6.660 1.00 68.86 B
ATOM 2766 N PRO B 72 18.645 24.091 -5.810 1.00 69.39 B
ATOM 2767 CD PRO B 72 19.604 25.212 -5.717 1.00 68.17 B
ATOM 2768 CA PRO B 72 17.794 24.047 -4.607 1.00 72.97 B
ATOM 2769 CB PRO B 72 18.441 25.093 -3.700 1.00 72.01 B
ATOM 2770 CG PRO B 72 18.980 26.106 -4.682 1.00 66.79 B
ATOM 2771 C PRO B 72 16.295 24.332 -4.802 1.00 76.33 B
ATOM 2772 O PRO B 72 15.906 25.212 -5.577 1.00 78.23 B
ATOM 2773 N THR B 73 15.465 23.549 -4.116 1.00 78.03 B
ATOM 2774 CA THR B 73 14.012 23.703 -4.165 1.00 79.80 B
ATOM 2775 CB THR B 73 13.321 22.561 -4.957 1.00 79.79 B
ATOM 2776 OG1 THR B 73 13.837 21.300 -4.526 1.00 76.35 B
ATOM 2777 CG2 THR B 73 13.516 22.726 -6.465 1.00 78.21 B

ATOM 2778 C THR B 73 13.476 23.736 -2.736 1.00 81.12 B
ATOM 2779 O THR B 73 14.259 23.731 -1.778 1.00 81.66 B
ATOM 2780 N GLU B 74 12.148 23.755 -2.608 1.00 82.48 B
ATOM 2781 CA GLU B 74 11.444 23.807 -1.323 1.00 83.30 B
ATOM 2782 CB GLU B 74 9.924 23.800 -1.552 1.00 86.76 B
ATOM 2783 CG GLU B 74 9.299 25.181 -1.759 1.00 88.22 B
ATOM 2784 CD GLU B 74 9.268 26.014 -0.480 1.00 88.90 B
ATOM 2785 OE1 GLU B 74 10.171 26.859 -0.297 1.00 91.28 B
ATOM 2786 OE2 GLU B 74 8.344 25.820 0.342 1.00 83.59 B
ATOM 2787 C GLU B 74 11.819 22.783 -0.247 1.00 82.77 B
ATOM 2788 O GLU B 74 12.549 23.122 0.684 1.00 82.37 B
ATOM 2789 N LYS B 75 11.369 21.538 -0.396 1.00 82.57 B
ATOM 2790 CA LYS B 75 11.648 20.512 0.606 1.00 82.95 B
ATOM 2791 CB LYS B 75 10.403 19.649 0.853 1.00 86.03 B
ATOM 2792 CG LYS B 75 10.022 19.554 2.334 1.00 92.10 B
ATOM 2793 CD LYS B 75 9.647 20.860 3.056 1.00 95.40 B
ATOM 2794 CE LYS B 75 9.730 20.880 4.582 1.00 95.86 B
ATOM 2795 NZ LYS B 75 11.138 20.730 5.068 1.00 94.83 B
ATOM 2796 C LYS B 75 12.889 19.640 0.418 1.00 81.66 B
ATOM 2797 O LYS B 75 13.170 18.782 1.265 1.00 82.98 B
ATOM 2798 N ASP B 76 13.652 19.889 -0.651 1.00 78.79 B
ATOM 2799 CA ASP B 76 14.881 19.134 -0.938 1.00 75.03 B
ATOM 2800 CB ASP B 76 15.397 19.440 -2.355 1.00 77.45 B
ATOM 2801 CG ASP B 76 14.915 18.435 -3.408 1.00 78.40 B
ATOM 2802 OD1 ASP B 76 14.634 17.266 -3.065 1.00 82.83 B
ATOM 2803 OD2 ASP B 76 14.852 18.809 -4.599 1.00 73.68 B
ATOM 2804 C ASP B 76 15.981 19.420 0.093 1.00 72.47 B
ATOM 2805 O ASP B 76 16.628 20.473 0.059 1.00 71.95 B
ATOM 2806 N GLU B 77 16.138 18.491 1.037 1.00 70.92 B
ATOM 2807 CA GLU B 77 17.135 18.594 2.108 1.00 69.88 B
ATOM 2808 CB GLU B 77 16.656 17.861 3.368 1.00 71.14 B
ATOM 2809 CG GLU B 77 15.403 18.457 4.010 1.00 73.93 B
ATOM 2810 CD GLU B 77 15.061 17.813 5.346 1.00 76.41 B
ATOM 2811 OE1 GLU B 77 15.306 18.453 6.394 1.00 75.73 B
ATOM 2812 OE2 GLU B 77 14.547 16.671 5.348 1.00 74.15 B
ATOM 2813 C GLU B 77 18.501 18.058 1.682 1.00 66.82 B
ATOM 2814 O GLU B 77 18.593 17.012 1.039 1.00 65.52 B
ATOM 2815 N TYR B 78 19.546 18.819 2.012 1.00 64.11 B

ATOM 2816 CA TYR B 78 20.937 18.478 1.694 1.00 59.21 B
ATOM 2817 CB TYR B 78 21.543 19.521 0.749 1.00 56.46 B
ATOM 2818 CG TYR B 78 20.929 19.547 -0.631 1.00 55.54 B
ATOM 2819 CD1 TYR B 78 19.816 20.367 -0.914 1.00 59.43 B
ATOM 2820 CE1 TYR B 78 19.211 20.373 -2.205 1.00 61.63 B
ATOM 2821 CD2 TYR B 78 21.438 18.733 -1.661 1.00 56.03 B
ATOM 2822 CE2 TYR B 78 20.847 18.730 -2.957 1.00 60.47 B
ATOM 2823 CZ TYR B 78 19.736 19.550 -3.217 1.00 61.76 B
ATOM 2824 OH TYR B 78 19.164 19.548 -4.470 1.00 66.36 B
ATOM 2825 C TYR B 78 21.794 18.371 2.960 1.00 57.39 B
ATOM 2826 O TYR B 78 21.484 18.996 3.981 1.00 61.03 B
ATOM 2827 N ALA B 79 22.871 17.584 2.880 1.00 52.75 B
ATOM 2828 CA ALA B 79 23.789 17.365 4.003 1.00 47.56 B
ATOM 2829 CB ALA B 79 23.198 16.325 4.973 1.00 48.06 B
ATOM 2830 C ALA B 79 25.192 16.932 3.569 1.00 44.84 B
ATOM 2831 O ALA B 79 25.458 16.744 2.377 1.00 42.46 B
ATOM 2832 N CYS B 80 26.085 16.805 4.552 1.00 39.84 B
ATOM 2833 CA CYS B 80 27.460 16.377 4.330 1.00 38.62 B
ATOM 2834 C CYS B 80 27.789 15.246 5.318 1.00 39.11 B
ATOM 2835 O CYS B 80 27.752 15.440 6.536 1.00 40.73 B
ATOM 2836 CB CYS B 80 28.420 17.558 4.500 1.00 36.59 B
ATOM 2837 SG CYS B 80 30.130 17.213 3.978 1.00 45.02 B
ATOM 2838 N ARG B 81 28.052 14.054 4.782 1.00 38.37 B
ATOM 2839 CA ARG B 81 28.366 12.871 5.585 1.00 35.95 B
ATOM 2840 CB ARG B 81 27.696 11.638 4.974 1.00 37.64 B
ATOM 2841 CG ARG B 81 27.763 10.378 5.811 1.00 44.66 B
ATOM 2842 CD ARG B 81 26.911 9.210 5.355 1.00 50.98 B
ATOM 2843 NE ARG B 81 27.251 8.797 3.996 1.00 56.79 B
ATOM 2844 CZ ARG B 81 26.380 8.326 3.107 1.00 56.77 B
ATOM 2845 NH1 ARG B 81 25.098 8.195 3.424 1.00 59.08 B
ATOM 2846 NH2 ARG B 81 26.784 8.041 1.876 1.00 59.61 B
ATOM 2847 C ARG B 81 29.871 12.701 5.617 1.00 36.05 B
ATOM 2848 O ARG B 81 30.514 12.697 4.568 1.00 36.53 B
ATOM 2849 N VAL B 82 30.425 12.572 6.825 1.00 36.04 B
ATOM 2850 CA VAL B 82 31.878 12.447 7.025 1.00 36.24 B
ATOM 2851 CB VAL B 82 32.457 13.755 7.692 1.00 38.45 B
ATOM 2852 CG1 VAL B 82 33.964 13.655 7.923 1.00 36.32 B
ATOM 2853 CG2 VAL B 82 32.155 14.988 6.839 1.00 39.19 B

ATOM 2854 C VAL B 82 32.299 11.239 7.871 1.00 34.02 B
ATOM 2855 O VAL B 82 31.785 11.039 8.963 1.00 36.26 B
ATOM 2856 N ASN B 83 33.288 10.496 7.375 1.00 34.47 B
ATOM 2857 CA ASN B 83 33.850 9.325 8.053 1.00 38.09 B
ATOM 2858 CB ASN B 83 33.729 8.073 7.177 1.00 41.95 B
ATOM 2859 CG ASN B 83 32.518 7.231 7.511 1.00 48.30 B
ATOM 2860 OD1 ASN B 83 32.378 6.741 8.641 1.00 53.26 B
ATOM 2861 ND2 ASN B 83 31.642 7.030 6.522 1.00 45.95 B
ATOM 2862 C ASN B 83 35.329 9.577 8.356 1.00 38.34 B
ATOM 2863 O ASN B 83 36.120 9.831 7.440 1.00 37.37 B
ATOM 2864 N HIS B 84 35.693 9.499 9.638 1.00 36.13 B
ATOM 2865 CA HIS B 84 37.073 9.715 10.086 1.00 34.47 B
ATOM 2866 CB HIS B 84 37.269 11.183 10.502 1.00 31.83 B
ATOM 2867 CG HIS B 84 38.703 11.586 10.679 1.00 30.87 B
ATOM 2868 CD2 HIS B 84 39.691 11.794 9.775 1.00 24.52 B
ATOM 2869 ND1 HIS B 84 39.267 11.803 11.921 1.00 27.57 B
ATOM 2870 CE1 HIS B 84 40.540 12.126 11.774 1.00 29.15 B
ATOM 2871 NE2 HIS B 84 40.824 12.126 10.481 1.00 32.78 B
ATOM 2872 C HIS B 84 37.338 8.792 11.270 1.00 35.88 B
ATOM 2873 O HIS B 84 36.393 8.356 11.926 1.00 43.07 B
ATOM 2874 N VAL B 85 38.617 8.530 11.558 1.00 34.38 B
ATOM 2875 CA VAL B 85 39.045 7.657 12.664 1.00 36.97 B
ATOM 2876 CB VAL B 85 40.614 7.448 12.647 1.00 40.04 B
ATOM 2877 CG1 VAL B 85 41.340 8.758 12.767 1.00 35.59 B
ATOM 2878 CG2 VAL B 85 41.083 6.477 13.747 1.00 38.03 B
ATOM 2879 C VAL B 85 38.554 8.096 14.055 1.00 37.89 B
ATOM 2880 O VAL B 85 38.384 7.268 14.947 1.00 41.24 B
ATOM 2881 N THR B 86 38.286 9.387 14.212 1.00 38.47 B
ATOM 2882 CA THR B 86 37.805 9.925 15.481 1.00 42.75 B
ATOM 2883 CB THR B 86 38.062 11.430 15.579 1.00 42.87 B
ATOM 2884 OG1 THR B 86 37.713 12.069 14.343 1.00 41.91 B
ATOM 2885 CG2 THR B 86 39.509 11.703 15.906 1.00 46.51 B
ATOM 2886 C THR B 86 36.321 9.660 15.722 1.00 44.64 B
ATOM 2887 O THR B 86 35.877 9.563 16.869 1.00 45.37 B
ATOM 2888 N LEU B 87 35.577 9.523 14.627 1.00 47.70 B
ATOM 2889 CA LEU B 87 34.137 9.276 14.659 1.00 52.47 B
ATOM 2890 CB LEU B 87 33.489 9.845 13.396 1.00 48.43 B
ATOM 2891 CG LEU B 87 33.787 11.305 13.053 1.00 45.92 B

ATOM 2892 CD1 LEU B 87 33.309 11.608 11.651 1.00 45.41 B
ATOM 2893 CD2 LEU B 87 33.142 12.234 14.055 1.00 44.88 B
ATOM 2894 C LEU B 87 33.794 7.790 14.782 1.00 57.43 B
ATOM 2895 O LEU B 87 34.378 6.945 14.090 1.00 61.07 B
ATOM 2896 N SER B 88 32.849 7.484 15.673 1.00 59.24 B
ATOM 2897 CA SER B 88 32.389 6.112 15.909 1.00 60.42 B
ATOM 2898 CB SER B 88 31.693 6.022 17.273 1.00 61.00 B
ATOM 2899 OG SER B 88 30.702 7.030 17.414 1.00 61.07 B
ATOM 2900 C SER B 88 31.433 5.703 14.782 1.00 60.39 B
ATOM 2901 O SER B 88 31.489 4.585 14.262 1.00 59.98 B
ATOM 2902 N GLN B 89 30.583 6.653 14.404 1.00 59.33 B
ATOM 2903 CA GLN B 89 29.606 6.489 13.339 1.00 59.63 B
ATOM 2904 CB GLN B 89 28.186 6.342 13.933 1.00 59.28 B
ATOM 2905 CG GLN B 89 27.726 7.482 14.849 1.00 61.70 B
ATOM 2906 CD GLN B 89 27.173 7.005 16.182 1.00 66.32 B
ATOM 2907 OE1 GLN B 89 27.388 5.855 16.592 1.00 63.96 B
ATOM 2908 NE2 GLN B 89 26.468 7.898 16.879 1.00 61.80 B
ATOM 2909 C GLN B 89 29.732 7.750 12.468 1.00 59.65 B
ATOM 2910 O GLN B 89 30.164 8.799 12.971 1.00 58.38 B
ATOM 2911 N PRO B 90 29.442 7.653 11.145 1.00 58.94 B
ATOM 2912 CD PRO B 90 29.132 6.465 10.329 1.00 58.85 B
ATOM 2913 CA PRO B 90 29.541 8.831 10.272 1.00 58.95 B
ATOM 2914 CB PRO B 90 29.058 8.299 8.915 1.00 57.07 B
ATOM 2915 CG PRO B 90 28.276 7.059 9.256 1.00 58.30 B
ATOM 2916 C PRO B 90 28.726 10.040 10.750 1.00 59.31 B
ATOM 2917 O PRO B 90 27.582 9.894 11.203 1.00 60.50 B
ATOM 2918 N LYS B 91 29.366 11.208 10.714 1.00 57.25 B
ATOM 2919 CA LYS B 91 28.756 12.457 11.151 1.00 57.44 B
ATOM 2920 CB LYS B 91 29.832 13.362 11.756 1.00 57.50 B
ATOM 2921 CG LYS B 91 29.345 14.365 12.792 1.00 58.86 B
ATOM 2922 CD LYS B 91 30.434 15.126 13.529 1.00 62.32 B
ATOM 2923 CE LYS B 91 30.016 16.025 14.675 1.00 70.29 B
ATOM 2924 NZ LYS B 91 31.208 16.620 15.345 1.00 74.58 B
ATOM 2925 C LYS B 91 28.045 13.173 10.007 1.00 56.95 B
ATOM 2926 O LYS B 91 28.646 13.434 8.965 1.00 58.81 B
ATOM 2927 N ILE B 92 26.756 13.449 10.203 1.00 56.09 B
ATOM 2928 CA ILE B 92 25.934 14.152 9.219 1.00 56.88 B
ATOM 2929 CB ILE B 92 24.600 13.376 8.849 1.00 57.41 B

ATOM 2930 CG2 ILE B 92 24.911 12.174 7.981 1.00 53.32 B
ATOM 2931 CG1 ILE B 92 23.734 13.020 10.087 1.00 67.54 B
ATOM 2932 CD1 ILE B 92 24.236 11.889 11.034 1.00 68.16 B
ATOM 2933 C ILE B 92 25.614 15.582 9.686 1.00 57.95 B
ATOM 2934 O ILE B 92 25.072 15.785 10.780 1.00 62.08 B
ATOM 2935 N VAL B 93 26.046 16.570 8.904 1.00 55.50 B
ATOM 2936 CA VAL B 93 25.790 17.980 9.214 1.00 54.35 B
ATOM 2937 CB VAL B 93 27.110 18.814 9.334 1.00 54.86 B
ATOM 2938 CG1 VAL B 93 26.801 20.297 9.601 1.00 48.52 B
ATOM 2939 CG2 VAL B 93 27.997 18.263 10.457 1.00 54.00 B
ATOM 2940 C VAL B 93 24.919 18.527 8.088 1.00 56.22 B
ATOM 2941 O VAL B 93 25.367 18.626 6.942 1.00 56.71 B
ATOM 2942 N LYS B 94 23.678 18.879 8.429 1.00 57.86 B
ATOM 2943 CA LYS B 94 22.703 19.407 7.468 1.00 57.36 B
ATOM 2944 CB LYS B 94 21.282 19.399 8.058 1.00 60.25 B
ATOM 2945 CG LYS B 94 20.646 18.020 8.220 1.00 67.80 B
ATOM 2946 CD LYS B 94 19.120 17.960 8.408 1.00 71.97 B
ATOM 2947 CE LYS B 94 18.504 18.509 9.697 1.00 72.95 B
ATOM 2948 NZ LYS B 94 18.775 17.649 10.888 1.00 71.19 B
ATOM 2949 C LYS B 94 23.022 20.804 6.950 1.00 55.43 B
ATOM 2950 O LYS B 94 23.748 21.570 7.591 1.00 56.02 B
ATOM 2951 N TRP B 95 22.503 21.106 5.762 1.00 54.01 B
ATOM 2952 CA TRP B 95 22.678 22.412 5.151 1.00 53.37 B
ATOM 2953 CB TRP B 95 22.710 22.313 3.617 1.00 49.79 B
ATOM 2954 CG TRP B 95 22.757 23.650 2.889 1.00 46.09 B
ATOM 2955 CD2 TRP B 95 21.858 24.098 1.869 1.00 46.45 B
ATOM 2956 CE2 TRP B 95 22.251 25.421 1.514 1.00 46.77 B
ATOM 2957 CE3 TRP B 95 20.752 23.514 1.211 1.00 47.92 B
ATOM 2958 CD1 TRP B 95 23.638 24.681 3.101 1.00 47.75 B
ATOM 2959 NE1 TRP B 95 23.336 25.745 2.283 1.00 45.99 B
ATOM 2960 CZ2 TRP B 95 21.572 26.180 0.524 1.00 48.69 B
ATOM 2961 CZ3 TRP B 95 20.069 24.268 0.216 1.00 49.51 B
ATOM 2962 CH2 TRP B 95 20.489 25.591 -0.112 1.00 49.34 B
ATOM 2963 C TRP B 95 21.515 23.274 5.607 1.00 56.85 B
ATOM 2964 O TRP B 95 20.352 22.977 5.315 1.00 58.10 B
ATOM 2965 N ASP B 96 21.853 24.308 6.370 1.00 60.23 B
ATOM 2966 CA ASP B 96 20.887 25.267 6.883 1.00 62.78 B
ATOM 2967 CB ASP B 96 21.165 25.528 8.369 1.00 65.30 B

ATOM 2968 CG ASP B 96 20.026 26.257 9.088 1.00 69.61 B
ATOM 2969 OD1 ASP B 96 19.757 25.894 10.256 1.00 72.50 B
ATOM 2970 OD2 ASP B 96 19.430 27.203 8.521 1.00 68.75 B
ATOM 2971 C ASP B 96 21.120 26.511 6.021 1.00 64.13 B
ATOM 2972 O ASP B 96 22.210 27.093 6.019 1.00 65.24 B
ATOM 2973 N ARG B 97 20.094 26.857 5.249 1.00 65.95 B
ATOM 2974 CA ARG B 97 20.093 27.996 4.324 1.00 68.99 B
ATOM 2975 CB ARG B 97 18.786 27.986 3.523 1.00 70.90 B
ATOM 2976 CG ARG B 97 18.441 26.633 2.907 1.00 72.55 B
ATOM 2977 CD ARG B 97 17.055 26.460 2.314 1.00 75.80 B
ATOM 2978 NE ARG B 97 16.700 27.546 1.400 1.00 77.59 B
ATOM 2979 CZ ARG B 97 15.907 27.416 0.337 1.00 79.58 B
ATOM 2980 NH1 ARG B 97 15.374 26.238 0.027 1.00 82.01 B
ATOM 2981 NH2 ARG B 97 15.635 28.476 -0.412 1.00 78.78 B
ATOM 2982 C ARG B 97 20.244 29.360 5.006 1.00 69.04 B
ATOM 2983 O ARG B 97 20.957 30.242 4.511 1.00 69.57 B
ATOM 2984 N ASP B 98 19.586 29.495 6.156 1.00 69.42 B
ATOM 2985 CA ASP B 98 19.576 30.722 6.952 1.00 69.10 B
ATOM 2986 CB ASP B 98 18.286 30.790 7.789 1.00 68.41 B
ATOM 2987 CG ASP B 98 17.024 30.820 6.933 1.00 65.33 B
ATOM 2988 OD1 ASP B 98 16.520 29.735 6.571 1.00 63.91 B
ATOM 2989 OD2 ASP B 98 16.532 31.927 6.631 1.00 63.15 B
ATOM 2990 C ASP B 98 20.797 30.915 7.859 1.00 69.23 B
ATOM 2991 O ASP B 98 20.948 31.972 8.478 1.00 69.50 B
ATOM 2992 N MET B 99 21.661 29.902 7.929 1.00 69.40 B
ATOM 2993 CA MET B 99 22.871 29.951 8.760 1.00 69.93 B
ATOM 2994 CB MET B 99 23.245 28.542 9.219 1.00 68.02 B
ATOM 2995 CG MET B 99 24.264 28.465 10.344 1.00 69.07 B
ATOM 2996 SD MET B 99 24.770 26.770 10.628 1.00 67.08 B
ATOM 2997 CE MET B 99 23.334 26.134 11.562 1.00 59.91 B
ATOM 2998 C MET B 99 24.049 30.575 8.006 1.00 70.32 B
ATOM 2999 O MET B 99 24.883 31.227 8.667 1.00 68.57 B
ATOM 3000 OXT MET B 99 24.131 30.389 6.770 1.00 72.21 B
ATOM 3001 C1 TWT D 2 57.390 23.811 -11.669 1.00 45.44 D
ATOM 3002 C2 TWT D 2 57.670 22.393 -11.230 1.00 51.36 D
ATOM 3003 C3 TWT D 2 56.465 21.509 -10.963 1.00 53.52 D
ATOM 3004 C4 TWT D 2 56.547 20.564 -9.772 1.00 54.41 D
ATOM 3005 C5 TWT D 2 55.564 20.779 -8.633 1.00 48.69 D

ATOM 3006 C6 TWT D 2 54.750 19.579 -8.191 1.00 45.72 D
ATOM 3007 C7 TWT D 2 54.691 19.272 -6.701 1.00 43.46 D
ATOM 3008 C8 TWT D 2 55.807 18.414 -6.120 1.00 40.49 D
ATOM 3009 C9 TWT D 2 55.479 17.561 -4.900 1.00 39.79 D
ATOM 3010 C10 TWT D 2 56.642 17.096 -4.030 1.00 35.75 D
ATOM 3011 C11 TWT D 2 56.914 17.880 -2.758 1.00 42.69 D
ATOM 3012 C12 TWT D 2 58.156 17.501 -1.955 1.00 46.22 D
ATOM 3013 C13 TWT D 2 58.933 18.601 -1.215 1.00 45.52 D
ATOM 3014 C14 TWT D 2 58.554 18.882 0.244 1.00 46.99 D
ATOM 3015 C15 TWT D 2 59.612 19.472 1.166 1.00 38.14 D
ATOM 3016 C16 TWT D 2 60.463 18.523 1.984 1.00 40.55 D
ATOM 3017 C17 TWT D 2 59.819 17.890 3.208 1.00 44.19 D
ATOM 3018 C18 TWT D 2 60.706 17.525 4.387 1.00 43.18 D
ATOM 3019 C19 TWT D 2 60.503 16.146 5.008 1.00 46.31 D
ATOM 3020 C20 TWT D 2 60.665 16.023 6.520 1.00 46.01 D
ATOM 3021 C21 TWT D 2 61.324 14.767 7.053 1.00 43.56 D
ATOM 3022 C22 TWT D 2 60.922 14.312 8.437 1.00 48.53 D
ATOM 3023 C1 SWT F 1 71.717 11.979 -6.552 1.00131.90 F
ATOM 3024 O1 SWT F 1 71.910 11.096 -5.488 1.00128.30 F
ATOM 3025 C2 SWT F 1 72.785 13.092 -6.548 1.00132.86 F
ATOM 3026 O2 SWT F 1 72.688 13.863 -5.356 1.00131.40 F
ATOM 3027 C3 SWT F 1 72.575 13.998 -7.767 1.00132.84 F
ATOM 3028 O3 SWT F 1 73.599 14.982 -7.822 1.00132.29 F
ATOM 3029 C4 SWT F 1 72.581 13.162 -9.055 1.00133.69 F
ATOM 3030 O4 SWT F 1 72.269 13.995 -10.166 1.00134.40 F
ATOM 3031 C5 SWT F 1 71.553 12.019 -8.953 1.00133.10 F
ATOM 3032 O5 SWT F 1 71.800 11.220 -7.771 1.00133.66 F
ATOM 3033 C6 SWT F 1 71.581 11.074 -10.151 1.00132.42 F
ATOM 3034 O6 SWT F 1 72.647 10.136 -10.064 1.00126.30 F
ATOM 3035 CL6 SWT F 1 65.105 16.994 -1.642 1.00 75.32 F
ATOM 3036 CL5 SWT F 1 66.321 16.767 -2.550 1.00 81.46 F
ATOM 3037 CL4 SWT F 1 65.985 15.837 -3.722 1.00 89.26 F
ATOM 3038 CL3 SWT F 1 66.537 14.430 -3.489 1.00 96.57 F
ATOM 3039 CL2 SWT F 1 67.222 13.895 -4.747 1.00104.40 F
ATOM 3040 CL1 SWT F 1 68.714 13.654 -4.495 1.00109.16 F
ATOM 3041 O SWT F 1 69.530 14.563 -4.659 1.00108.27 F
ATOM 3042 N SWT F 1 68.996 12.508 -3.861 1.00112.40 F
ATOM 3043 CB2 SWT F 1 69.682 11.376 -4.526 1.00115.41 F

ATOM 3044 CB1 SWT F 1 71.210 11.514 -4.339 1.00120.42 F
ATOM 3045 CR1 SWT F 1 69.160 10.028 -3.974 1.00110.88 F
ATOM 3046 OR SWT F 1 69.695 9.779 -2.669 1.00112.29 F
ATOM 3047 CR2 SWT F 1 67.618 9.964 -3.937 1.00104.53 F
ATOM 3048 CR3 SWT F 1 67.037 10.705 -2.721 1.00 95.83 F
ATOM 3049 CR4 SWT F 1 66.848 9.757 -1.534 1.00 91.36 F
ATOM 3050 CR5 SWT F 1 67.291 10.412 -0.225 1.00 88.01 F
ATOM 3051 CR6 SWT F 1 66.088 10.776 0.650 1.00 83.08 F
ATOM 3052 CR7 SWT F 1 66.016 12.289 0.873 1.00 80.52 F
ATOM 3053 CR8 SWT F 1 65.305 12.619 2.176 1.00 75.19 F
ATOM 3054 CR9 SWT F 1 65.863 13.759 3.016 1.00 73.28 F
ATOM 3055 CR10 SWT F 1 65.378 15.174 2.727 1.00 72.01 F
ATOM 3056 CR11 SWT F 1 64.936 16.009 3.921 1.00 70.49 F
ATOM 3057 CR12 SWT F 1 65.284 17.488 3.910 1.00 72.63 F
ATOM 3058 CR13 SWT F 1 66.045 18.043 5.111 1.00 74.72 F
ATOM 3059 CR14 SWT F 1 67.468 18.532 4.865 1.00 79.65 F
ATOM 3060 CR15 SWT F 1 67.996 19.642 5.765 1.00 82.49 F
ATOM 3061 CR16 SWT F 1 68.643 20.840 5.094 1.00 81.68 F
ATOM 3062 CL7 SWT F 1 64.085 17.934 -2.295 1.00 72.09 F
ATOM 3063 CL8 SWT F 1 63.211 18.611 -1.251 1.00 69.84 F
ATOM 3064 CL9 SWT F 1 63.284 20.134 -1.160 1.00 65.16 F
ATOM 3065 CL10 SWT F 1 62.371 20.934 -2.079 1.00 60.18 F
ATOM 3066 CL11 SWT F 1 62.511 22.448 -2.058 1.00 53.57 F
ATOM 3067 CL12 SWT F 1 61.307 23.246 -2.532 1.00 48.80 F
ATOM 3068 CL13 SWT F 1 61.542 24.651 -3.026 1.00 40.57 F
ATOM 3069 CL14 SWT F 1 61.707 24.797 -4.508 1.00 37.53 F
ATOM 3070 CL15 SWT F 1 60.454 25.077 -5.288 1.00 32.76 F
ATOM 3071 CL16 SWT F 1 60.630 25.439 -6.738 1.00 30.20 F
ATOM 3072 CL17 SWT F 1 60.228 24.407 -7.754 1.00 33.69 F
ATOM 3073 CL18 SWT F 1 59.647 24.927 -9.026 1.00 34.28 F
ATOM 3074 OH2 WAT S 2 42.437 20.412 0.022 1.00 35.65 S
ATOM 3075 OH2 WAT S 3 53.094 15.104 10.333 1.00 27.31 S
ATOM 3076 OH2 WAT S 4 33.716 30.014 10.501 1.00 15.62 S
ATOM 3077 OH2 WAT S 5 49.193 19.185 -17.084 1.00 31.00 S
ATOM 3078 OH2 WAT S 6 42.373 19.959 -6.918 1.00 30.87 S
ATOM 3079 OH2 WAT S 7 48.550 17.560 -2.066 1.00 32.78 S
ATOM 3080 OH2 WAT S 8 59.484 14.016 -16.309 1.00 18.35 S
ATOM 3081 OH2 WAT S 9 49.570 24.297 1.265 1.00 23.45 S

ATOM 3082 OH2 WAT S 10 32.173 34.424 -7.680 1.00 4.37 S
ATOM 3083 OH2 WAT S 11 44.840 17.521 -9.337 1.00 20.74 S
ATOM 3084 OH2 WAT S 12 20.436 14.835 3.162 1.00 28.97 S
ATOM 3085 OH2 WAT S 13 38.712 49.435 8.538 1.00 27.66 S
ATOM 3086 OH2 WAT S 14 49.118 5.938 6.699 1.00 39.82 S
ATOM 3087 OH2 WAT S 15 39.880 27.701 -10.681 1.00 25.86 S
ATOM 3088 OH2 WAT S 16 47.416 15.671 -3.910 1.00 19.43 S
ATOM 3089 OH2 WAT S 17 25.674 42.441 -2.943 1.00 29.65 S
ATOM 3090 OH2 WAT S 19 24.770 29.564 2.661 1.00 30.73 S
ATOM 3091 OH2 WAT S 20 41.015 27.077 2.253 1.00 40.18 S
ATOM 3092 OH2 WAT S 21 54.479 21.295 17.281 1.00 28.10 S
ATOM 3093 OH2 WAT S 22 36.925 46.454 -9.092 1.00 21.15 S
ATOM 3094 OH2 WAT S 24 45.732 41.064 -2.081 1.00 30.90 S
ATOM 3095 OH2 WAT S 25 51.874 26.461 -17.841 1.00 26.20 S
ATOM 3096 OH2 WAT S 26 40.106 31.619 -11.887 1.00 32.47 S
ATOM 3097 OH2 WAT S 27 42.925 22.512 8.538 1.00 34.79 S
ATOM 3098 OH2 WAT S 28 66.807 23.047 -11.935 1.00 33.57 S
ATOM 3099 OH2 WAT S 30 35.735 10.720 -0.617 1.00 16.73 S
ATOM 3100 OH2 WAT S 31 49.354 14.273 -5.122 1.00 21.36 S
ATOM 3101 OH2 WAT S 36 37.461 4.328 14.610 1.00 26.91 S
ATOM 3102 OH2 WAT S 37 31.064 48.776 20.335 1.00 26.22 S
ATOM 3103 OH2 WAT S 38 39.419 23.835 11.381 1.00 23.73 S
ATOM 3104 OH2 WAT S 42 50.501 34.662 -19.238 1.00 20.32 S
ATOM 3105 OH2 WAT S 43 27.883 24.679 8.563 1.00 31.47 S
ATOM 3106 OH2 WAT S 46 19.071 35.135 -5.226 1.00 26.48 S
ATOM 3107 OH2 WAT S 47 50.999 21.470 15.352 1.00 34.63 S
ATOM 3108 OH2 WAT S 48 32.407 31.536 7.666 1.00 20.23 S
ATOM 3109 OH2 WAT S 49 18.121 47.897 10.834 1.00 34.61 S
ATOM 3110 OH2 WAT S 50 56.307 7.289 16.176 1.00 26.67 S
ATOM 3111 OH2 WAT S 51 44.551 35.789 -2.442 1.00 10.71 S
ATOM 3112 OH2 WAT S 52 47.918 16.451 -6.563 1.00 8.65 S
ATOM 3113 OH2 WAT S 53 74.597 12.531 -0.845 1.00 42.09 S
ATOM 3114 N1 DTI D 7 71.254 6.982 -6.846 1.00104.35 D
ATOM 3115 CN4 DTI D 7 69.974 6.871 -6.117 1.00103.31 D
ATOM 3116 CN5 DTI D 7 71.040 7.778 -8.065 1.00102.10 D
ATOM 3117 CN3 DTI D 7 71.721 5.634 -7.232 1.00102.63 D
ATOM 3118 C2 DTI D 7 72.564 6.911 -4.677 1.00100.45 D
ATOM 3119 C1 DTI D 7 72.279 7.664 -6.000 1.00101.42 D

ATOM 3120 C3 DTI D 7 72.890 7.890 -3.542 1.00100.53 D
ATOM 3121 C4 DTI D 7 72.820 7.226 -2.166 1.00 97.68 D
ATOM 3122 C5 DTI D 7 71.485 7.283 -1.424 1.00 94.46 D
ATOM 3123 C6 DTI D 7 71.371 8.220 -0.225 1.00 89.40 D
ATOM 3124 C7 DTI D 7 70.225 7.953 0.746 1.00 86.05 D
ATOM 3125 C8 DTI D 7 69.996 8.956 1.870 1.00 86.12 D
ATOM 3126 C9 DTI D 7 69.760 8.402 3.274 1.00 85.94 D
ATOM 3127 C10 DTI D 7 68.882 9.219 4.213 1.00 84.41 D
ATOM 3128 C11 DTI D 7 68.448 8.573 5.526 1.00 84.95 D
ATOM 3129 C12 DTI D 7 67.089 8.990 6.100 1.00 85.47 D
ATOM 3130 C13 DTI D 7 66.608 8.276 7.366 1.00 85.28 D
ATOM 3131 C14 DTI D 7 65.111 8.265 7.674 1.00 80.47 D
ATOM 3132 C15 DTI D 7 64.698 8.019 9.124 1.00 77.01 D
ATOM 3133 C16 DTI D 7 63.275 8.346 9.529 1.00 72.98 D
END

Supplementary Information - Statistics for data collection and refinement

Data Collection	**CD1b/GM2**	**CD1b/PI**
Resolution range (Å)	100-2.8	25-2.2
Completeness (%) (outer)	88.8 (71.1)	92.3 (89.8)
Total observations	89500	334867
Unique reflections	13203	27623
Average I/σ(I) (outer)	13.7 (1.8)	39.1 (15.8)
R_{merge} (%) (outer)	10.3 (32.5)	5.1 (20.6)

Model refinement	**CD1b/GM2**	**CD1b/PI**
Maximum resolution	2.80	2.26
Number of reflections (working set/ test set)	12383/535	24656/751
R_{work}/R_{free} (%)	22.4/27.5	20.3/23.3
r.m.s deviations from standard stereochemistry		
Bonds (Å)	0.012288	0.007716

Angles (°)	1.72965	1.47377
Number of atoms		
Protein	3000	3005
Ligand(s)	85	90
Waters	40	232
NO_3	0	12
Ramachandran plot		
Most favoured (%)	88.5	89.4
Additional (%)	11.2	9.3
Generous (%)	0.3	1.2
Disallowed (%)	0	0

Values in parentheses refer to the highest resolution shells (the outer shell is between 2.91-2.80Å and between 2.28-2.20Å for the CD1b/GM2 the CD1b/PI data respectively).

$$R_{merge} = \frac{\sum_h \sum_i \left| I_i(h) - \langle I(h) \rangle \right|}{\sum_h \sum_i \left| I(h) \right|}$$

where $I_i(h)$ is the ith measurement of reflection h and $\langle I(h) \rangle$ is the weighted mean of all measurements of h.

$$R = \frac{\sum_h \left| F_{obs} - F_{calc} \right|}{\sum_h F_{obs}}$$

where F_{obs} and F_{calc} are the observed and calculated structure factor amplitudes respectively. R_{work} and R_{cryst} were calculated using the working and test set, respectively.

CLAIMS

1. A method of producing a CD1/ligand complex said method comprising the steps of:

a) obtaining a denatured CD1 protein;

b) contacting said denatured CD1 protein with ligand in an environment comprising detergent; and

c) isolating said CD1/ligand complex.

2. A method according to claim 1 wherein the denatured CD1 protein is also reduced.

3. A method according to claim 1 or claim 2 wherein the ligand is a lipid.

4. A method according to claim 3 wherein the lipid is a glycolipid or a phospholipid.

5. The method of claim 4 wherein said phospholipid is phosphatidylinositol.

6. The method of claim 4 wherein said glycolipid is ganglioside GM2 or alpha-galactosylceramide.

7. A method according to claim 3 or claim 4 wherein the lipid has between 10 and 80 carbon atoms.

8. A method according to any one of the preceding claims wherein the detergent is selected from the group consisting of a single chain detergent, such as acyclic single carbonyl chain detergents with acyl chain length C2-C60; sphingosines; ceramides with truncated alkyl chains; diacylglycerol-type lipids with truncated alkyl

chains; and triacylglycerol-type lipids with truncated alkyl chains.

9. A method according to any one of the preceding claims wherein the detergent is cetyltrimethylammonium bromide (CTAB).

10. A method according to any one of the preceding claims comprising the further step of removing excess detergent from the environment prior to isolation of the CD1/ligand complex.

11. A method according to claim 9 wherein the excess detergent is removed using a cyclodextrin.

12. A method according to any one of the preceding claims wherein the CD1 molecule is CD1b, CD1c or CD1d.

13. A method according to claim 12 wherein the CD1 molecule is CD1b.

14. A method according to any one of the preceding claims, wherein the CD1 protein contains at least one biotinylation site.

15. A method according to any one of the preceding claims, wherein the CD1 protein is complexed with the Fc portion of an immunoglobulin.

16. A method as claimed in any preceding claim, further comprising the step of forming a multimer comprising a plurality of said CD1/ligand complexes.

17. The method of claim 16, wherein said multimer is a dimer, trimer or tetramer.

18. A method as claimed in any preceding claim, further comprising the step of labelling the CD1 protein with a chemical marker.

19. The method of claim 18, wherein said marker is a fluorescent compound.

20. A method according to any one of claims 1 to 17 further comprising the step of producing a pharmaceutical composition comprising the CD1/ligand complex and a pharmaceutically acceptable carrier.

21. A CD1/ligand complex produced by a method according to any one of the preceding claims for use in a method of medical treatment.

22. A method of medical treatment comprising the step of administering a therapeutically effective amount of a CD1/ligand complex produced by the method of any of claims 1 to 20.

23. Use of a CD1/ligand complex produced by a method according to any of claims 1 to 20 in the preparation of a medicament for treating infectious diseases caused by parasites, mycobacteria, fungi, and bacteria; tumours or autoimmune diseases.

24. Use of a CD1/ligand complex produced by a method according to any of claims 1 to 20 for detection of

lipid-specific T-lymphocytes, wherein said ligand is a lipid.

25. Use of a CD1/ligand complex comprising CD1d/alpha-galactosylceramide produced by a method according to any of claims 1 to 20 for detection of mammalian T-lymphocytes.

26. A method of inducing or boosting an immune response in an individual to a lipid antigen, said method comprising administering a CD1/ligand complex to said individual wherein the ligand in the CD1/ligand complex is said lipid antigen.

27. A method according to claim 26, wherein said CD1/ligand complex has been produced by a method according to any one of claims 1 to 20.

28. A method for detecting a T-cell specific for a lipid antigen, said method comprising the steps of

(a) contacting a CD1/ligand complex with a biological sample suspected of comprising said T-cell; wherein said CD1/ligand complex comprises the lipid antigen; and

(b) detecting the presence of a T-cell specific for the lipid antigen following interaction between the T-cell and the CD1/ligand complex.

29. A method according to claim 28 wherein said T-cell is associated with a disease state.

30. A method according to claim 28 or 29 which is carried out *in vitro*.

31. A crystal of CD1/ligand complex.

32. A crystal as claimed in claim 31 wherein said ligand is a lipid.

33. A crystal as claimed in claim 32 wherein said lipid is a glycolipid, or a phospholipid.

34. A crystal of CD1/ligand complex having unit cell dimensions of a = 87.5 Å ± 5%, b = 177 Å ± 5% c = 75 Å ± 5%.

35. A crystal structure according to claim 34 having the three dimensional atomic co-ordinates of Table 1.

36. A crystal as claimed in any of claims 31 to 35 wherein said ligand is phosphatidylinositol (PI) or ganglioside GM2.

37. A crystal as claimed in any of claims 31 to 36 wherein the CD1 molecule is CD1b, CD1c or CD1d.

38. A crystal as claimed in claim 37 wherein the CD1 is CD1b.

39. A method for growing a crystal of CD1/ligand complex as claimed in any of claims 31 to 38 comprising growing the crystal by sitting drop crystallisation using a precipitant comprising 0.2M Lithium Nitrate and 20% w/v Polyethylene Glycol.

40. A computer-based method of rational drug design comprising the steps of:

providing the structure of the CD1/ligand complex as defined by the coordinates of Table 1;

providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the structure of the CD1/ligand complex of Table 1.

41. A computer-based method of rational drug design comprising the steps of:

providing the coordinates of at least two atoms of the CD1 of Table 1;

providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the selected coordinates of the CD1.

42. A computer-based method of rational drug design as claimed in claim 40 or 41, wherein said candidate modulator molecule comprises a plurality of molecular fragments, said step of fitting the structure of the candidate modulator molecule further comprising the step of:

assembling the molecular fragments to form said candidate modulator molecule.

43. The method of any of claims 40 to 42 which further comprises the steps of:

obtaining or synthesising the candidate modulator molecule;

contacting the candidate modulator molecule with CD1; and

determining the ability of the candidate modulator molecule to interact with CD1.

44. The method of any of claims 40 to 42 which further comprises the steps of:

obtaining or synthesising the candidate modulator molecule;

forming a complex of CD1 and said candidate modulator molecule; and

analysing said complex by X-ray crystallography to determine the ability of said candidate modulator molecule to interact with CD1.

45. A compound having a chemical structure selected using the method of any of claims 40 to 44.

46. The compound of claim 45, wherein said compound inhibits or enhances the presentation of ligand by CD1.

47. A machine readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by all or a portion of the structure coordinates of CD1/ligand complex according to Table 1.

48. Use of the machine readable data storage medium according to claim 47 to design modulators of the CD1/ligand complex.

49. A computer system intended to generate structures of, and/or perform rational drug design for, CD1/ligand

complex, or complexes of CD1/ligand with a potential modulator, the system containing machine readable data comprising

(1) atomic coordinate data of Table 1, said data defining the three dimensional structure of CD1/ligand complex, or at least one sub-domain of the three-dimensional structure of CD1/ligand complex, or the coordinates of at least two atoms of CD1/ligand complex; or

(2) structure factor data for CD1/ligand complex, said structure factor data being derivable from the atomic coordinate data of Table 1.

50. A method of generating structures of, and/or performing rational drug design for, CD1/ligand complex, or complexes of CD1/ligand with a potential modulator, comprising the step of operating a computer containing machine readable data comprising

(1) atomic coordinate data of Table 1, said data defining the three dimensional structure of CD1/ligand complex, or at least one sub-domain of the three-dimensional structure of CD1/ligand complex, or the coordinates of at least two atoms of CD1/ligand complex; or

(2) structure factor data for CD1/ligand complex, said structure factor data being derivable from the atomic coordinate data of Table 1.

51. A method of identifying a candidate modulator molecule of CD1/ligand complex comprising the steps of:

providing the structure, or at least one sub-domain, of the CD1/ligand complex of Table 1;

characterising at least one active site of CD1; and

identifying a candidate modulator molecule for interaction with said active site.

52. A method of identifying a candidate modulator molecule of CD1/ligand complex as claimed in claim 51, wherein said step of identifying a candidate modulator molecule comprises the step of:

designing a candidate modulator molecule to interact with said active site.

53. A method of identifying a candidate modulator molecule of CD1/ligand complex as claimed in claim 51, wherein said step of identifying a candidate modulator molecule comprises the steps of:

screening a plurality of candidate modulator molecules for interaction with the characterised active site; and

selecting at least one interacting candidate modulator molecule.

54. A candidate modulator molecule as identified by the method of any of claims 51 to 53, wherein said candidate modulator molecule interacts with a plurality of said active sites.

55. A method of assessing the ability of a candidate modulator molecule to interact with CD1 or CD1/ligand complex comprising the steps of:

obtaining or synthesising said candidate modulator molecule;

forming a crystallised composite of CD1 or CD1/ligand complex and said candidate modulator; and

analysing the composite by X-ray crystallography to determine the ability of the candidate modulator to interact with CD1 or CD1/ligand complex.

56. The method as claimed in claim 55, wherein the composite diffracts X-rays for the determination of atomic coordinates of the composite to a resolution of better than 2Å.

57. The method of claim 55 or 56 wherein said crystallised composite is formed by crystal soaking or co-crystallisation.

58. A method of determining three dimensional structures of CD1 or CD1/ligand complex homologues or analogues of unknown structure comprising the steps of:

aligning a representation of an amino acid sequence of a CD1 or CD1/ligand complex homologue or analogue of unknown structure with the amino acid sequence of CD1 or CD1/ligand complex to match homologous regions of amino acid sequences;

modelling the structure of the matched homologous regions of the homologue or analogue of unknown structure on the structure as defined in Table 1 of the corresponding regions of CD1 or CD1/ligand complex; and

determining a conformation for the homologue or analogue of unknown structure which substantially preserves the structure of said matched homologous regions.

59. A method for determining the structure of a protein comprising the steps of:

providing the coordinates of Table 1; and

positioning said coordinates in the crystal unit cell of said protein so as to provide a structure for said protein.

60. A method for determining the structure of a compound bound to CD1/ligand complex comprising the steps of:

providing a crystal of CD1/ligand complex; and

soaking the crystal with the compound to form a complex; and

determining the structure of the complex by employing the data of Table 1.

Fig.1a.

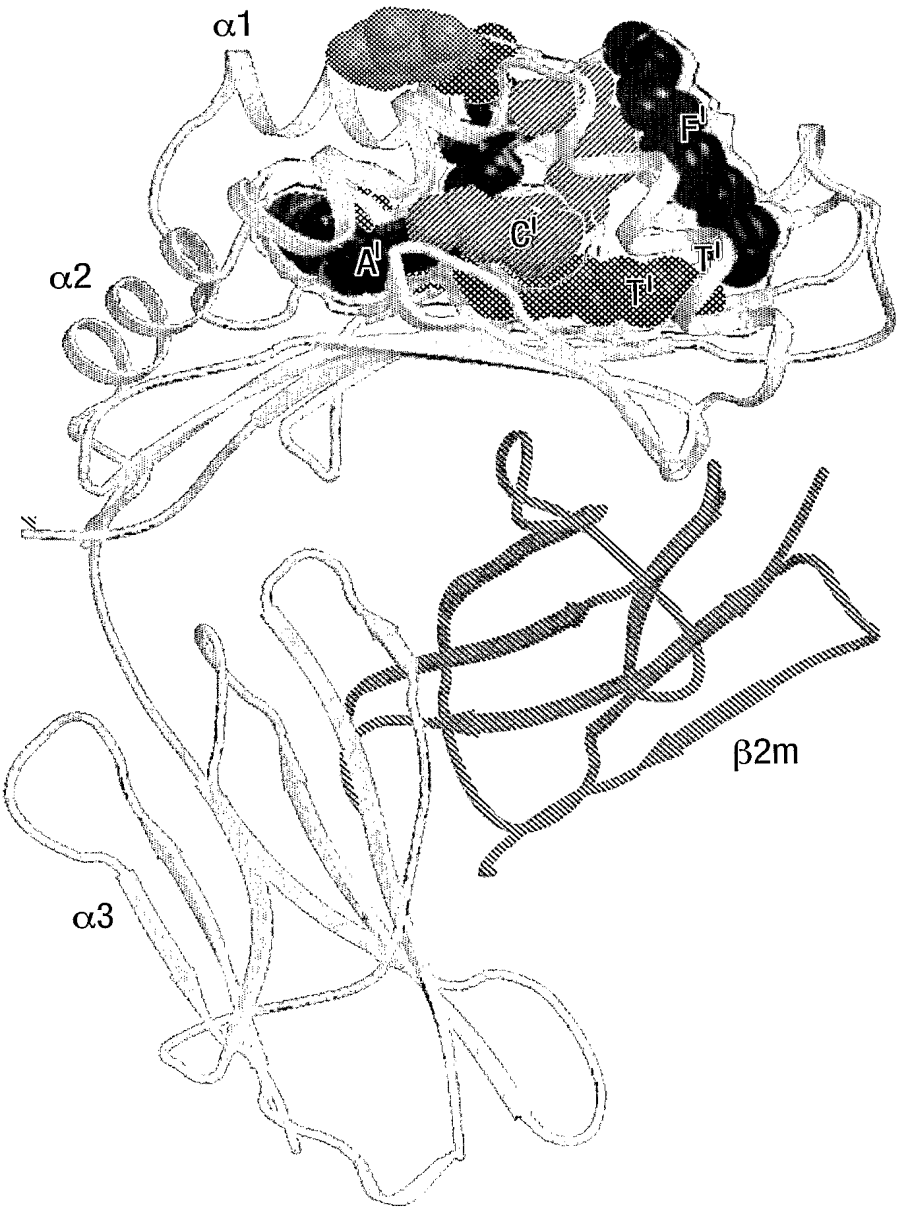


Fig.1a (Cont).

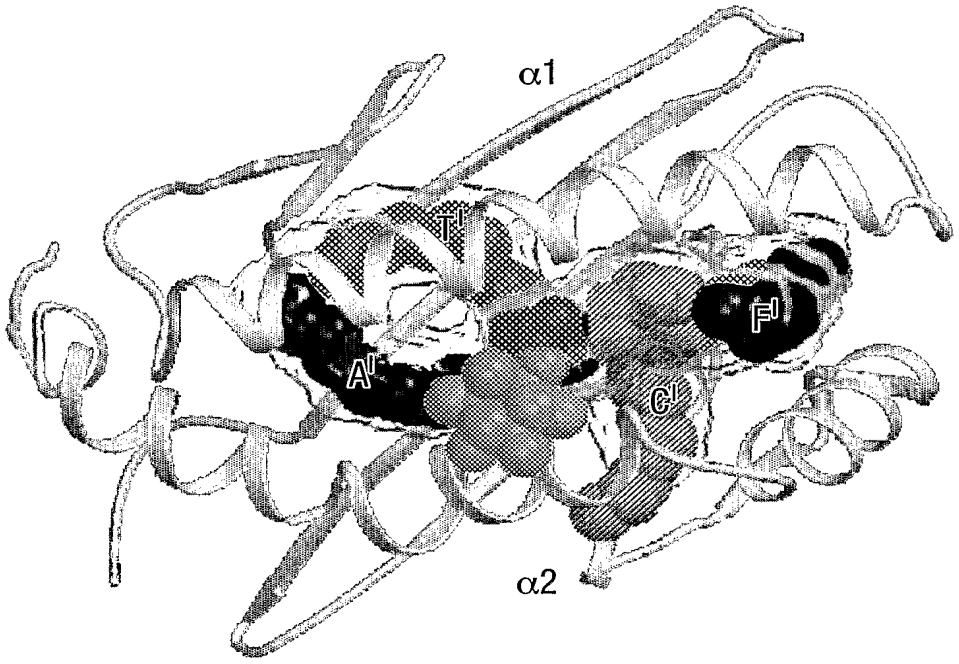


Fig.1b.

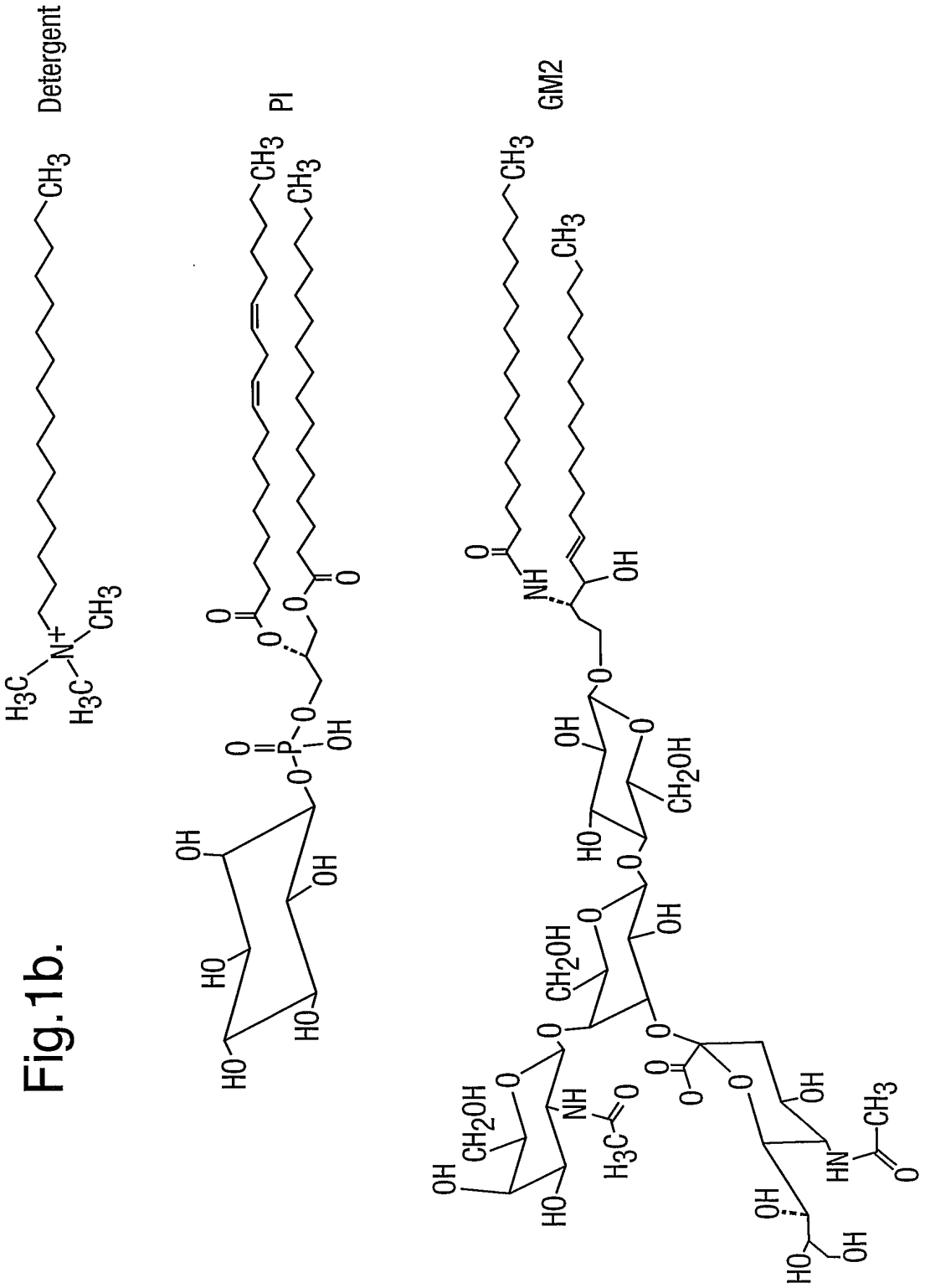


Fig.2a.

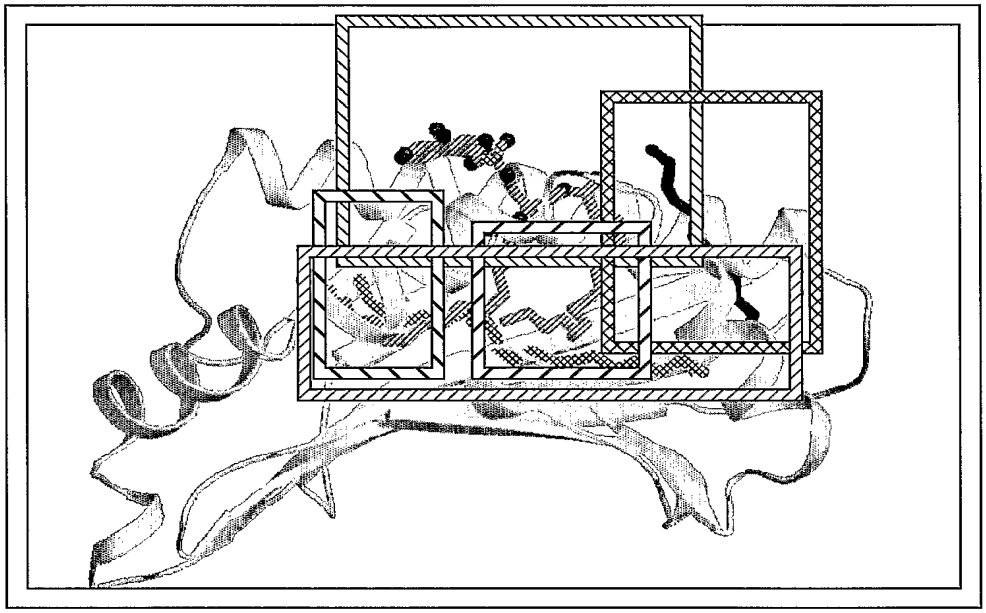


Fig.2b.

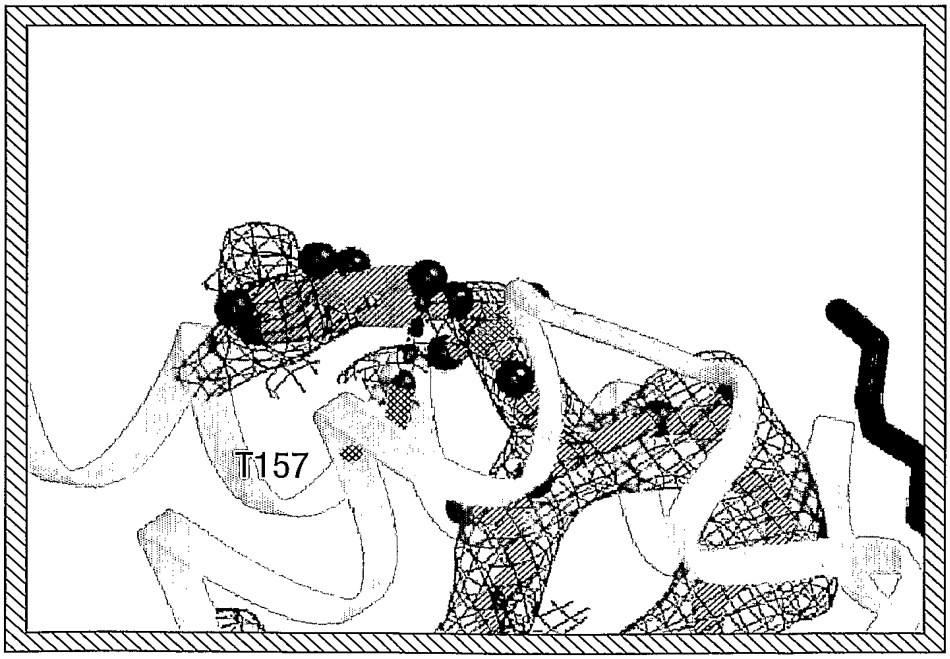


Fig.2c.

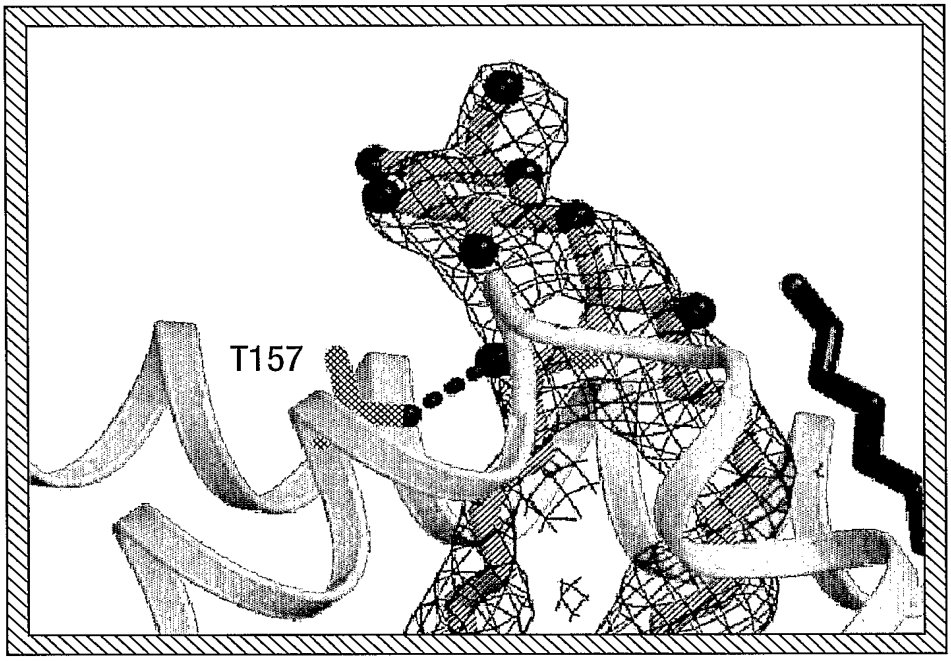


Fig.2d.

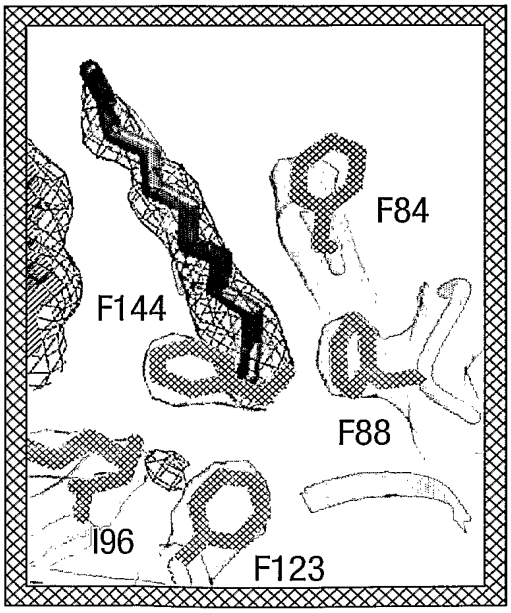


Fig.2e.

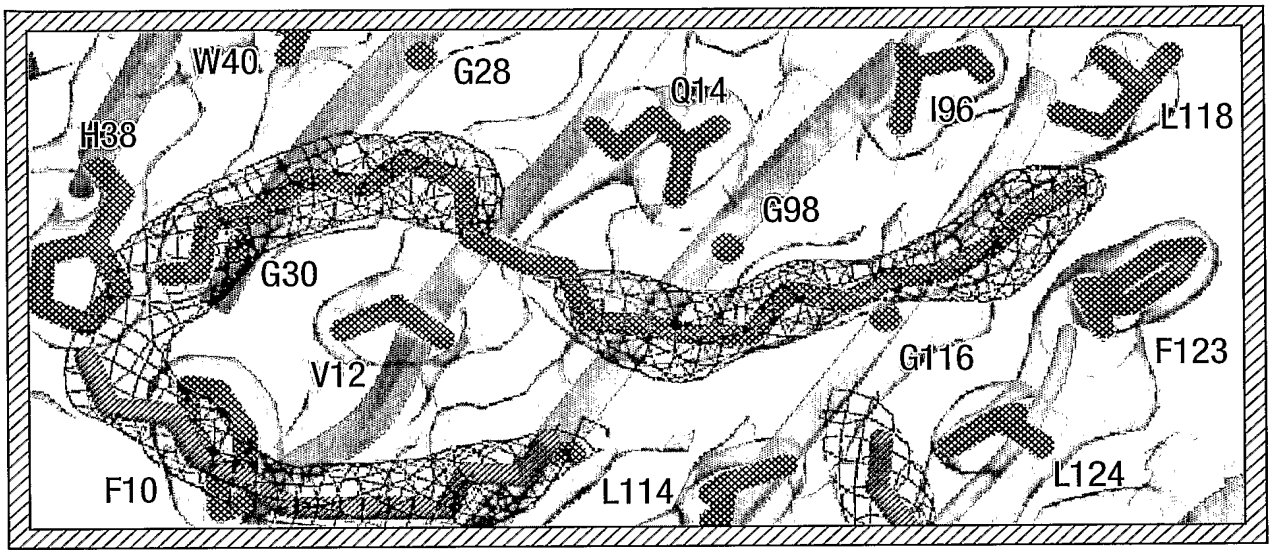


Fig.2f.

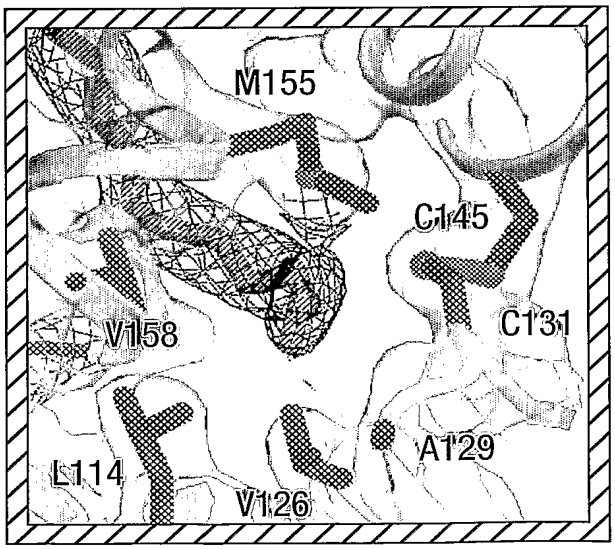


Fig.2g.

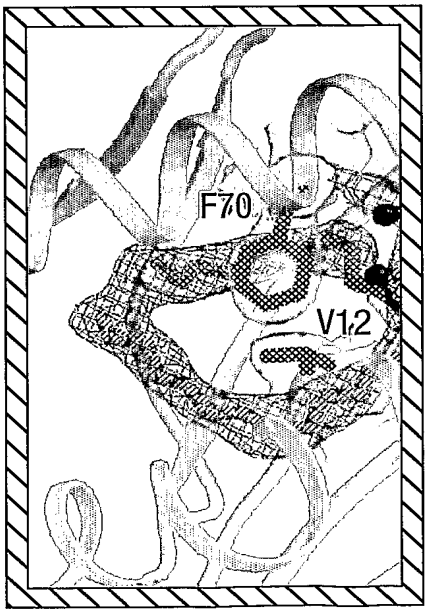


Fig.3a.

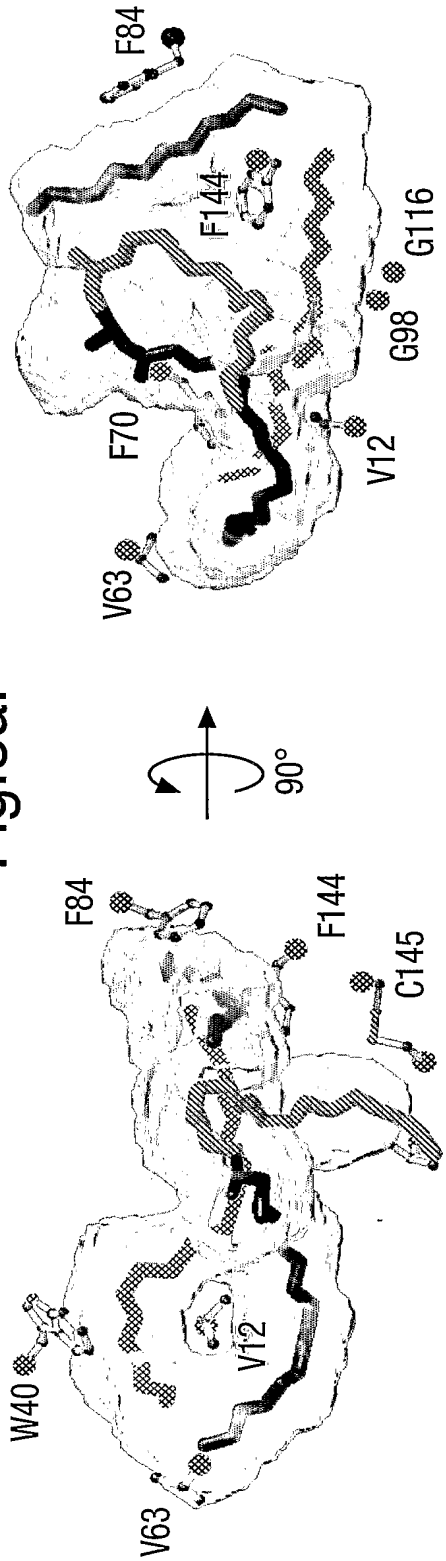

F84
F144
C145
C131
W40
V12
V63
90°
F84
F144
G116
G98
F70
V12
V63

Fig.3b.

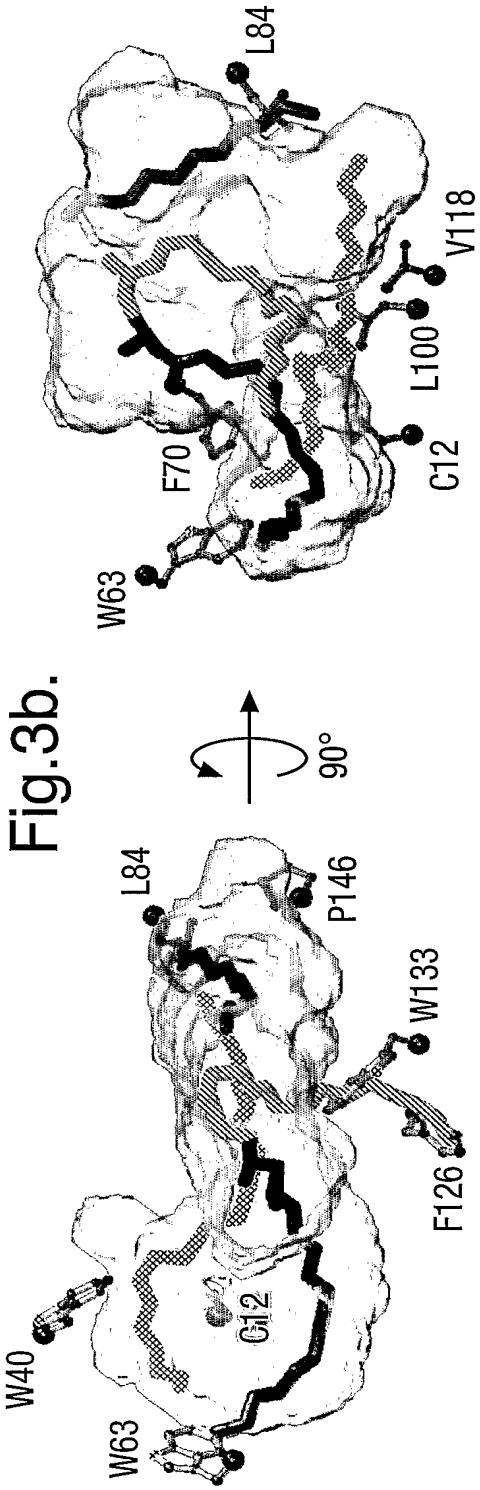

L84
P146
W133
F126
W40
G12
W63
90°
L84
V118
L100
C12
F70
W63

Fig.3c.

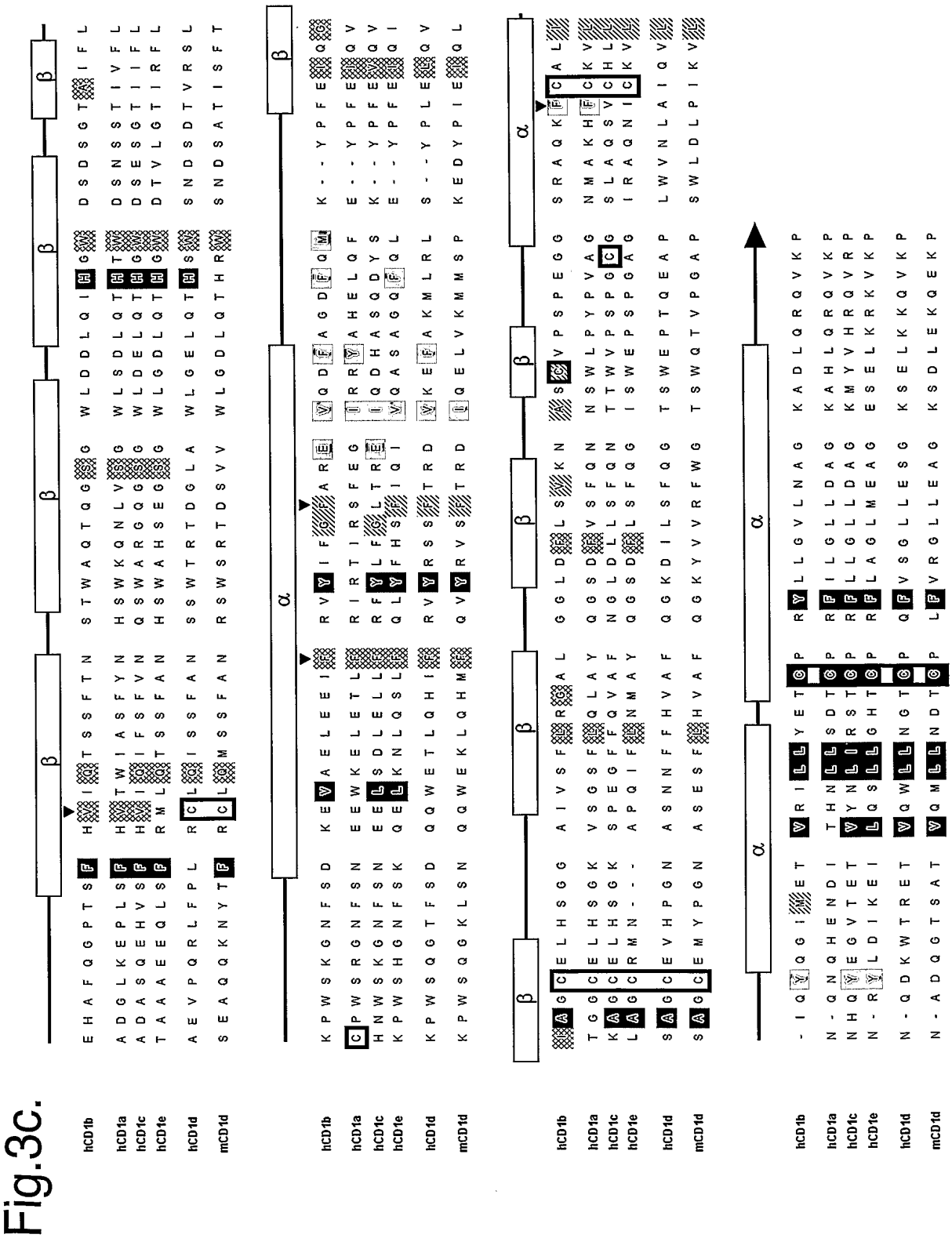
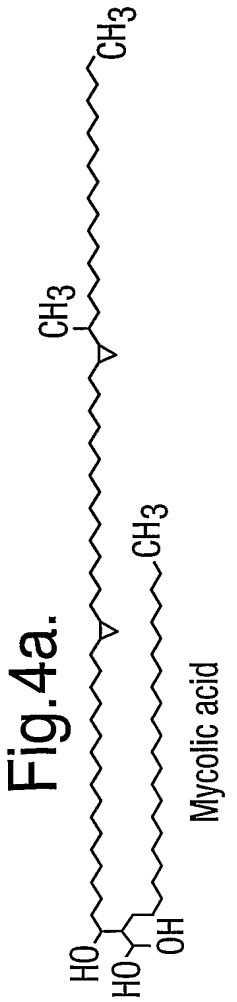
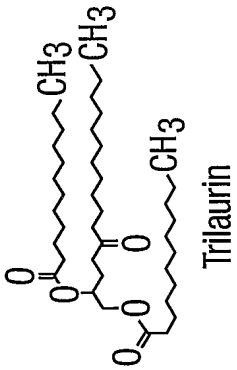


Fig.4a.

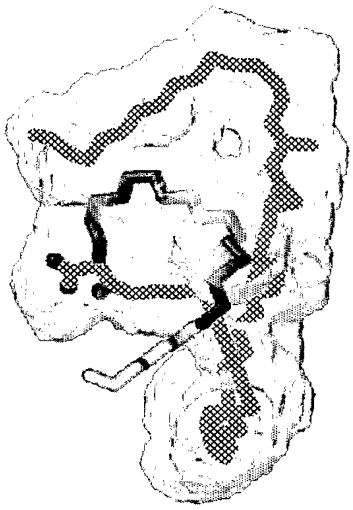


Mycolic acid



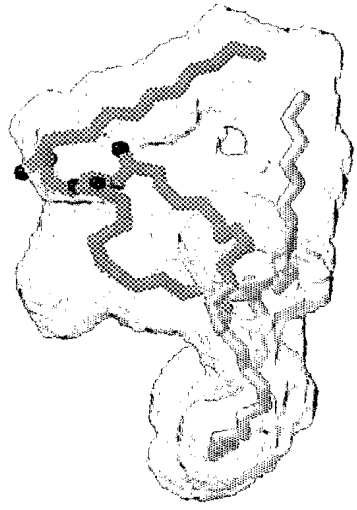
Trilaurin

Fig.4b.

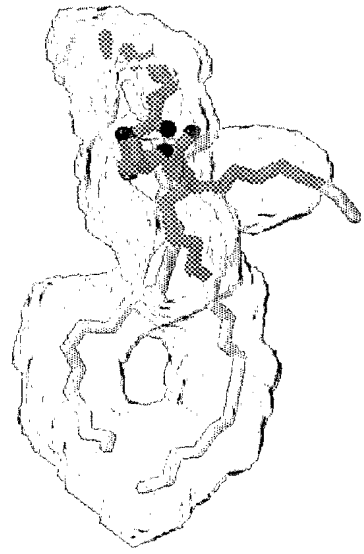


90°

Fig.4c.



90°



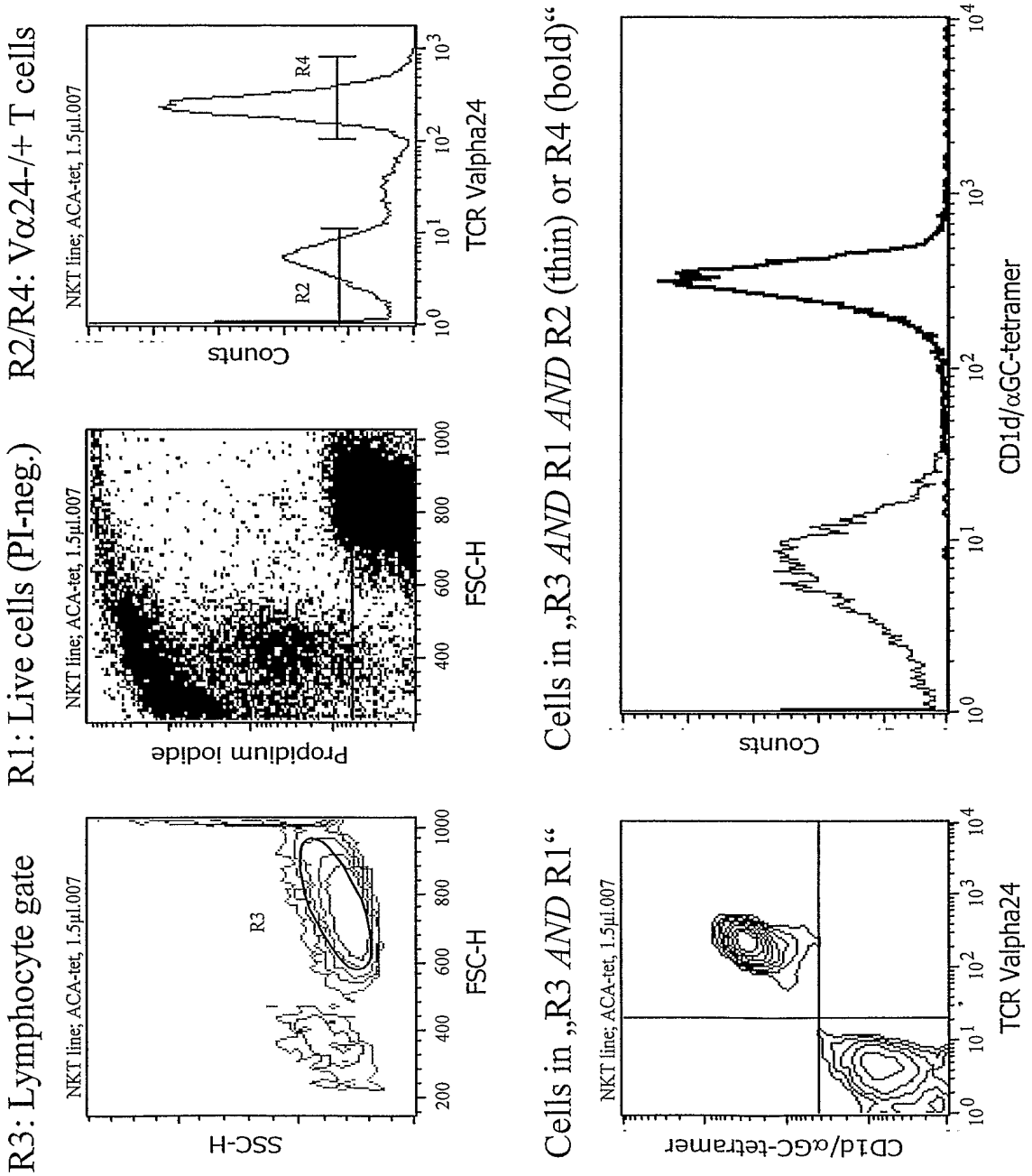

A
B
C
R3: Lymphocyte gate
R1: Live cells (PI-neg.)
R2/R4: Vα24-/+ T cells
NKT line; ACA-tet, 1.5µl.007
SSC-H
FSC-H
R3
Propidium Iodide
Counts
R2
R4
TCR Valpha24
Cells in „R3 AND R1"
Cells in „R3 AND R1 AND R2 (thin) or R4 (bold)"
CD1d/αGC-tetramer
D
E

Figure 5